Getting Started

Varian NMR Spectrometer Systems
With VNMR 6.1B Software

Pub. No. 01-999083-00, Rev. A1298

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Varian NMR spectrometer systems running VNMR 6.1B software

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Overview of Contents

SAFETY PRECAUTIONS **17**

Introduction **21**

Chapter 1. **Overview of Varian NMR** **23**

Chapter 2. **VNMR Basics** **39**

Chapter 3. **Using *GLIDE*** ***53***

Chapter 4. **Using the VNMR Menu System** **59**

Chapter 5. **Using the Command Mode** **93**

Chapter 6. **Preparing for an Experiment** **101**

Chapter 7. **Acquiring Data** **183**

Chapter 8. **Data Processing** **221**

Chapter 9. **Display, Plotting, and Printing** **231**

Chapter 10. **Storing, Retrieving, and Moving Data** **275**

Glossary **295**

Index **299**

Table of Contents

SAFETY PRECAUTIONS **17**

Introduction **21**

Chapter 1. **Overview of Varian NMR** **23**

1.1 Varian NMR Spectrometer System 23
Host Computer 23
NMR System Console 24
Superconducting Magnet and Probe 25
1.2 User Interface 25
VNMR Software 25
Mouse, Keyboard, and Remote Status Module 27
VNMR Display Screen 27
Using Multiple Windows 28
1.3 Advanced Features 29
Queuing 30
Multitasking 30
Experiments 31
Multiple Related FIDs 31
Multiple Unrelated Sets of Data 32
MAGICAL II Macro Language 32
Optional Specialized Software 33
1.4 Introduction to UNIX and VNMR Files 33
UNIX File System 34
VNMR Directories and Files 34
NMR System Administrator and Other Users 36
Paths and the Working Directory 37
User Library 38

Chapter 2. **VNMR Basics** **39**

2.1 Entering and Exiting VNMR 39
To Start VNMR 39
To Exit VNMR 40
2.2 Working with VNMR on the Host Computer 41
Mouse Device 41
Mouse Buttons 42
Keyboard 42
Remote Status Module 43
VNMR Display Screen 44
Standard Windows 44
Optional Windows 48

Chapter 3. **Using *GLIDE*** ***53***

3.1 Activating *GLIDE* *53*

Opening *GLIDE* 53
Closing *GLIDE* 53
3.2 Using *GLIDE* 54
Running a Standard Experiment 54
Customizing a 1D Experiment 55
3.3 Customizing Combination Experiments 56
Processing and Plotting Combination Experiments 57
Walkup NMR 58

Chapter 4. Using the VNMR Menu System 59

4.1 Working With Menus 60
Interactive Programs with Menus 60
4.2 Customizing the Menu System 64
4.3 Menu System Step-by-Step 64
4.4 Permanent Menu 65
4.5 Main Menu 66
4.6 Workspace Menu 67
4.7 Setup Menus 67
Setup Menu 67
Nucleus Selection Menu 68
Solvent Selection Menu 68
1D Pulse Sequence Setup Menu 68
1D Pulse Sequence Setup Secondary Menu 69
2D Pulse Sequence Setup Menu 69
2D Pulse Sequence Setup Secondary Menu 70
Applications Mode Menu 70
4.8 Acquire Menu 70
4.9 Processing Menus 71
1D Data Processing Menu 71
Interactive 1D FID Display Menu—df Program 71
1D Processing Parameter Setup Menu 72
Interactive Weighting Menu—wti Program 72
Interactive 1D Spectrum Display Menu—ds Program 73
2D Data Processing Menu 73
2D Processing Parameter Setup Menu 73
2D Interferogram Processing Menu 74
Interactive 2D Color Map Display Main Menu—dconi Program 74
Interactive 2D Display Projection Menu—dconi Program 75
Interactive 2D Peak Picking Main Menu—ll2d Program 75
2D Peak Picking Automatic Menu—ll2d Program 75
2D Peak Picking Edit Menu—ll2d Program 76
2D Peak Picking File Menu—ll2d Program 76
2D Peak Picking Display Menu—ll2d Program 76
4.10 Display Menus 77
1D Data Display Menu 77
1D Data Manipulation Menu 77
1D Display Size Selection Menu 78
1D Plotting Menu 78
1D Data Display Secondary Menu 78

2D Data Display Menu 79
2D Display Size Selection Menu 79
2D Data Manipulation Menu 79
2D Plotting Menu 80
2D Data Display Secondary Menu 80
4.11 Analyze Menus 81
Analyze Menu 81
Exponential Analysis Menu 81
Automatic DEPT Analysis Menu 81
Automatic COSY Analysis Menu 82
Add/Subtract Menu 82
Interactive Add/Subtract Menu—addi Program 83
Spin Simulation Main Menu 83
Spin Simulation First Definition Menu 83
Spin Simulation Second Definition Menu 84
Spin Simulation Third Definition Menu 84
Spin Simulation Secondary Menu 84
Spin Simulation Line Assignment Menu 85
Deconvolution Menu 85
Regression 1 Menu 86
Regression 2 Menu 86
Regression 3 Menu 86
4.12 File Menus 87
Files Main Menu 87
Directory Menu 88
Directory Secondary Menu 88
Files Information Menu 89
Files Tape Menu 89
Files Data Menu 90
Files Data Secondary Menu 90
Files Secondary Menu 90
4.13 Secondary Main Menu 91
Pulse Sequence Entry Main Menu 91
Configuration Menu 92

Chapter 5. Using the Command Mode 93

5.1 Commands 93
Command Entry 94
Command Arguments 94
5.2 Parameters 94
Parameter Entry 95
Parameter Display 96
Parameter Value Limitations 96
Parameter Entry Limitations 96
5.3 Command Line Editing and Reentry 96
5.4 Macro Automation 98

Chapter 6. Preparing for an Experiment 101

6.1 Preparing the Sample 101
Solvent Selection 101

Sample Height 101
Sample Position 102
Sample Tubes 103
6.2 Ejecting and Inserting the Sample 103
To Eject a Sample, Without a Sample Changer 104
To Insert a Sample, Without a Sample Changer 105
To Change a Sample, With a Sample Changer 106
6.3 Retrieving Parameter Sets 106
Location of Parameter Sets 107
To List Parameter Sets 108
To Recall Any Parameter Set 109
To Recall Standard Parameter Sets 110
To Create Selected Parameters 111
To List Parameter Groups 112
6.4 Removing and Inserting the Probe 112
To Remove the Probe 112
To Insert the Probe 113
6.5 Using Probe Files and Templates 113
6.6 Tuning the Probe 113
To Tune Probes on UNITY*INOVA* and UNITY*plus* *114*
Tuning Probes on *MERCURY-VX*, *MERCURY, GEMINI 2000* *124*
Tunning Probes on UNITY and VXR-S Systems 126
6.7 Spinning the Sample 127
6.8 Optimizing Lock 130
Lock Power, Gain, and Phase 131
Lock Control Methods 132
Leaving Lock in the Current State 132
Running an Experiment Unlocked 132
Simple Autolock 132
Optimizing Autolock 133
Full Optimization 134
Lock Level and Spin Speed Error Handling 134
Lock Loop Time Constant Control 135
6.9 Adjusting Shims 135
Shim Gradients 135
Methods of Shimming 136
Keyboard Entry 136
Saving and Retrieving Shim Values 137
Manual Emulation Shimming 138
Automated Shimming 139
Shimming Criteria for Autoshim 140
Shim Methods for Autoshim 140
User-Defined Shim Methods for Autoshim 142
Interactive Autoshim 143
Fully Automatic Autoshim 144
Background Autoshim 145
Hardware Autoshim 145
Gradient Autoshim 146
Which Shims to Use on a Routine Basis 147

Shimming Different Sample Geometries 147
6.10 Using the Acquisition Window 148
Opening the Window 148
Connecting to the Acquisition System 149
Making a Choice in a Display 150
Changing Parameter Values 150
LOCK Display 151
Using lockfreq to Find Lock Resonance 152
Using sethw to Set Lock Frequency 153
Simple Locking 153
FID/Spectrum Shimming Windows 154
Interactive Parameter Adjustment 159
Shimming on the FID 160
Shimming on the Spectrum 160
SHIM Display 161
6.11 Shimming Using the Ultra•nmr Shim System 164
Hardware Overview 164
Interface Box 164
Shimming 166
Installing the First Probe 166
Floppy Disk Use 166
Enabling the Acquisition Window 167
Turning the System Off and On 167
6.12 Gradient Autoshimming 168
Gradient Shimming Method 169
Configuring Gradients and Hardware Control 169
Mapping the Shims 169
Shimmap Files and Parameters 172
Automated Shimming 172
Deuterium Gradient Shimming 174
Homospoil Gradient Shimming for ^{1}H or ^{2}H 174
Full Deuterium Gradient Shimming Procedure for Lineshape 175
General User Gradient Shimming 176
Suggestions for Improving Results 176
Gradient Shimming Menus 177

Chapter 7. Acquiring Data 183

7.1 Setting Frequency-Related Parameters 183
Frequency Setting 183
Transmitter and Decoupler Positioning 184
Spectral Window 185
7.2 Setting Pulse-Sequence-Related Parameters 185
Standard Two-Pulse Parameters 187
Commands for Setting Parameters 188
The “Status” Concept 190
Observe Transmitter and Decoupling Parameters 190
Decoupler Modes 193
Temperature-Related Control 195
Temperature-Related Parameters 196
Pulsed Field Gradient Related Parameters 196

7.3 Creating and Editing Experiment Text Files 197
Creating and Editing a Text File 197
Displaying and Handling a Text File 197
7.4 Performing Acquisition 198
Initiating Acquisition 198
Shimming During an Acquisition 200
Queueing Acquisitions 200
Chained Acquisition 201
Stopping and Resuming Acquisition 202
Pausing, Halting, and Aborting Acquisition 202
Data Precision and Overflow 203
Automatic Processing 203
Acquisition Status Window 204
Receiver Gain 205
Homospoil 206
File Protection 206
Remote Acquisition 207
Acquisition Information 208
Acquisition Status Codes 208
VNMR Error Messages 209
Noise Level Analysis 209
7.5 Applying Digital Filtering 209
Types of Digital Filtering 210
Control of DSP 210
Inline DSP 211
Real-Time DSP 213
Postacquisition DSP 217
Removing Quadrature Artifacts Using DSP 218
To Apply Frequency-Shifted Quadrature Detection 218

Chapter 8. Data Processing 221

8.1 Weighting Function 221
8.2 Interactive Weighting 223
8.3 Fourier Transformation 223
8.4 Phasing 224
Phase Parameters 224
Autophase Algorithm 225
Spectrum Display 225
8.5 Advanced Data Processing 226
FID Phase Rotation 226
Frequency Shifting 227
Data Processing Methods 227
Linear Prediction 227
Solvent Subtraction Filtering 228
Interleave FIDs 229

Chapter 9. Display, Plotting, and Printing 231

9.1 Interactive FID and Spectrum Display 231
Display Parameters 232
Plotting 232

9.2 Interactive FID Display 233
FID Display Menu 233
Controlling Cursors and FID Intensity 234
Interactive FID Windowing 235
Interactive Phasing Mode 235
9.3 Stacked and Whitewashed FID Display and Plotting 236
Stacked FIDs 236
Whitewashed FIDs 237
9.4 Interactive Spectrum Display 237
Interactive 1D Spectrum Display Menus 238
Controlling the Cursors and Spectral Intensity 239
Interactive Spectral Windowing Mode 240
Interactive Phasing Mode 240
Interactive Integral Reset Mode 241
Interactive Zero- and First-Order Base Correction Mode 241
Setting the Integral Value 242
Setting the Reference Position 242
Interactive Inset Display 242
9.5 Spectral Display and Plotting 243
Display Parameters 243
Vertical Scale Adjustment 245
Line Listings 246
Line Resolution 247
Referencing 247
Spectral Plotting 249
Display Limits 250
9.6 Integration 250
Displaying Integrals Step-by-Step 250
Baseline Correction 252
Integral Reset Points 253
Integral Regions 253
Integral Display and Plotting 253
9.7 Plotting 254
Plotter Output 254
Plotter Configuration 255
Plotter Resolution and Speed 256
Selecting a Plotter 257
Color Printing 257
Plotting Parameter Lists and Text Files 261
9.8 Plot Designer 262
System Requirement 262
Starting Plot Designer 262
Customizing a Plot 263
Adjusting and Restoring Plot Parameters 269
Moving Objects and Changing Object Size 270
Changing the Shape of the Plot Designer Window 270
Changing the Size of the Plot Designer Window 270
Saving Your Plot 270
Printing Your Plot 270

Getting Help 270
Exiting Plot Designer 271
9.9 Printing 271
9.10 User-Controllable Line Drawing 272

Chapter 10. Storing, Retrieving, and Moving Data 275

10.1 Working with Directories and Files 275
Default Directory 275
Creating and Manipulating Directories 276
Creating and Manipulating Files 276
10.2 Storing Data 277
Experiment Files 277
Saving Data 277
Saving Parameters 278
Saving Shim Coil Settings 278
10.3 Retrieving Data 279
Using rt, rtp, and rts to Retrieve Files 279
Using *GLIDE* to Retrieve Data 280
Using CDE File Manager to Retrieve Data 280
Correcting Saved Parameter Sets 280
User-Written FID Files 281
10.4 Transferring Data Using Ethernet and limNET 281
Transferring Data Using Ethernet 282
Transferring Data Using limNET 282
File Suffixes 283
Initiating Transfers from a Remote Node 284
Error Messages from limNET 285
10.5 Converting Data Between Systems 286
Converting Text Files 286
Converting Data Files 287
Decomposing a Library 287
Step-by-Step Example with limNET 288
Converting Bruker Data 289
10.6 Magnetic Tape Operations 289
Reading Tapes from Gemini, VXR-4000, and XL Systems 290
Reading Bruker Data Files from 9-Track Tape 290
Sharing a Tape on a Network 291
Moving Data to PCs and Macintoshes via Floppy Disk 291
10.7 Compressing Data 292
Compressing and Uncompressing FID Data Files 292
Compressing Digitally Filtered FID Files 293
Compressing Double-Precision VNMR FID Data 293

Glossary 295

Index 299

List of Figures

Figure 1. Magnet, Probe, and Associated Electronics 26
Figure 2. VNMR Display Screen 27
Figure 3. *GLIDE* User Interface 28
Figure 4. CDE Toolbar 28
Figure 5. Windows Menu 29
Figure 6. FontSelect Window 29
Figure 7. File Structure Overview 35
Figure 8. Remote Status Module 43
Figure 9. VNMR Display Screen 44
Figure 10. Status Window and Input Window 45
Figure 11. Menu System Buttons 46
Figure 12. Typical Parameter Display in `dg` Program 47
Figure 13. CONSOLE and VNMR Shell Windows 48
Figure 14. *GLIDE* User Interface Window 49
Figure 15. Workspace Menu under OpenWindows 49
Figure 16. CDE Toolbar 50
Figure 17. Icons for Closed VNMR Windows 51
Figure 18. *GLIDE* User Interface Window 53
Figure 19. COSY Customization Window 57
Figure 20. HMQC Customization Window 57
Figure 21. Sample Depth Indicator 103
Figure 22. TUNE INTERFACE Panel 114
Figure 23. Probe Tuning Window (`qtune` Program) 117
Figure 24. Minimal Display Mode for the Tune Display 118
Figure 25. Tune Control Panel (`qtune` Program) 119
Figure 26. Pull-Down Menu for Center Frequencies 119
Figure 27. Pull-Down Menu For Span 120
Figure 28. Cursor and Grid Controls 120
Figure 29. Pull-Down Menu for Marker 1 121
Figure 30. Scale Controls 121
Figure 31. Tune Calibration Window 122
Figure 32. Help Pull-Down Menu 124
Figure 33. Spin Information in LOCK Display (`acqi` Program) 127
Figure 34. Spinner Control Window (`spinner` Program) 128
Figure 35. Acqmeter Lock Displays (`acqmeter` Program) 130
Figure 36. Lock Frequency Acquisition Window 134
Figure 37. Acquisition Window (`acqi` Program) 149
Figure 38. Abbreviated Acquisition Window 149
Figure 39. LOCK Display Window (`acqi` Program) 151
Figure 40. Finding Lock 153

Figure 41. Opening Style 1 FID/Spectrum Display Window (`acqi` Program) 154
Figure 42. Style 2 FID Shimming Display in Real-time (`acqi` Program) 155
Figure 43. Autoshim Method Editor Panel (`acqi` Program) 158
Figure 44. Spectrum in FID/Spectrum Display Window (`acqi` Program) 159
Figure 45. Spectrum Display Window with IPA (`acqi` Program) 160
Figure 46. SHIM Display Window (`acqi` Program) 161
Figure 47. Auto Mode Window (`acqi` Program) 162
Figure 48. Ultra•nmr Shim. System Interface Controls and Display 165
Figure 49. Shimmap Plot 171
Figure 50. Curve Fit Plot 173
Figure 51. Display of Shim Adjustments for Each Iteration 173
Figure 52. Positioning the Spectral Window 185
Figure 53. Acquisition Parameters for Standard Two-Pulse Sequence 187
Figure 54. Graphical Pulse Sequence Display (`dps` Program) 189
Figure 55. Display Properties Panel (`dps` Program) 189
Figure 56. Property Button Window (`dps` Program) 190
Figure 57. Logical Periods A, B, C in Standard Two-Pulse Sequence 190
Figure 58. Attenuator Configurations (Part 1 of 2) 191
Figure 59. Attenuator Configurations (Part 2 of 2) 192
Figure 60. Temperature Control Window 196
Figure 61. Acquisition Window (`acqi` Program) 200
Figure 62. SHIM Window During Acquisition (`acqi` Program) 201
Figure 63. Acquisition Status Window (`acqstat` Program) 204
Figure 64. Acqstatus Setup Window (`Acqstatus` Program) 206
Figure 65. Digital Filters Compared to Analog Filters 214
Figure 66. Interactive FID Display (`df` Program) 233
Figure 67. Interactive Spectrum Display (`ds` program) 238
Figure 68. Color Selection Window (`color` Program) 258
Figure 69. 2D Phase Color Selection Window (`color` Program) 259
Figure 70. 2D Absolute Value Selection Window 259
Figure 71. Image Color Selection Window 260
Figure 72. Plot Designer Window 262
Figure 73. Window Preferences Panel 263
Figure 74. Window with Data and Without Borders and a Grid 264
Figure 75. Region Editor Window 266
Figure 76. `menu` File 267
Figure 77. Item Preferences Window 268
Figure 78. Text Input Window 269
Figure 79. Plot Save Window 270

List of Tables

Table 1. Entering and Exiting VNMR 39
Table 2. VNMR Interface and Display Tools 42
Table 3. VNMR Menu System (Part 1 of 4) 61
Table 3. VNMR Menu System (Part 2 of 4) 62
Table 3. VNMR Menu System (Part 3 of 4) 63
Table 3. VNMR Menu System (Part 4 of 4) 64
Table 4. Special Keys for VNMR Line Editing 97
Table 5. Automated Acquisition Macros 98
Table 6. Automated Calibration Macros 98
Table 7. Automated Plotting Macros 99
Table 8. Automated Processing Macros 99
Table 9. Sample Tube Depths 102
Table 10. Sample Changing Commands and Parameters 104
Table 11. Retrieving Parameter Sets Commands and Parameters 107
Table 12. Probe File Macros and Parameters 113
Table 13. Probe Tuning Commands 113
Table 14. Sample Spinning Commands and Parameters 128
Table 15. Lock Commands and Parameters 131
Table 16. Homogeneity Adjustment Commands and Parameters 137
Table 17. Permissible Shimming Criterion Values 140
Table 18. Codes for Standard Shim Gradient Combinations 141
Table 19. Hexadecimal Codes for Shim Groups 143
Table 20. Interactive Acquisition Commands and Parameters 148
Table 21. Gradient Shim Availability 168
Table 22. Gradient Shimming Commands and Parameters 169
Table 23. Typical ^{2}H Gradient Shimming Parameters for Common Solvents 174
Table 24. Acquisition Frequency-Related Commands and Parameters 184
Table 25. Acquisition Pulse-Sequence-Related Commands and Parameters 186
Table 26. Experiment Text File Commands 197
Table 27. Commands and Parameters for Acquiring Data 199
Table 28. Fields in the Acquisition Status Window (acqstat Program) 205
Table 29. Digital Filtering Commands and Parameters 211
Table 30. Maximum Values for `sw*oversamp` and `np*oversamp` 212
Table 31. Weighting and Fourier Transform Commands, Macros, and Parameters 222
Table 32. Phasing Spectra Commands and Parametersn 224
Table 33. Advanced Data Processing Commands and Parameters 226
Table 34. Interactive FID Display Commands and Parameters 233
Table 35. FID Display and Plotting Commands and Parameters 236
Table 36. Interactive Spectrum Display Commands and Parameters 238
Table 37. Spectral Display Commands and Parameters 244

Table 38. Spectral Plotting Commands and Parameters 245
Table 39. Integral Display and Plotting Commands and Parameters 251
Table 40. Plotting Commands and Parameters 254
Table 41. Window Preference Controls 263
Table 42. Plot Designer Tools 265
Table 43. Region Editor Buttons 267
Table 44. Printer-Associated Commands and Parameters 271
Table 45. User-Controllable Line Drawing Commands 273
Table 46. Directory and File Handling Commands and Parameters 276
Table 47. Data Storage Commands and Parameters 277
Table 48. Data Retrieval Commands and Parameters 279
Table 49. Ethernet and limNET Data Transfer Commands 281
Table 50. Data Conversion Commands 287
Table 51. Magnetic Tape Operations Commands 289

SAFETY PRECAUTIONS

The following warning and caution notices illustrate the style used in Varian manuals for safety precaution notices and explain when each type is used:

WARNING: ***Warnings*** **are used when failure to observe instructions or precautions could result in injury or death to humans or animals, or significant property damage.**

CAUTION: ***Cautions*** **are used when failure to observe instructions could result in serious damage to equipment or loss of data.**

Warning Notices

Observe the following precautions during installation, operation, maintenance, and repair of the instrument. Failure to comply with these warnings, or with specific warnings elsewhere in Varian manuals, violates safety standards of design, manufacture, and intended use of the instrument. Varian assumes no liability for customer failure to comply with these precautions.

WARNING: **Persons with implanted or attached medical devices such as pacemakers and prosthetic parts must remain outside the 5-gauss perimeter of the magnet.**

The superconducting magnet system generates strong magnetic fields that can affect operation of some cardiac pacemakers or harm implanted or attached devices such as prosthetic parts and metal blood vessel clips and clamps.

Pacemaker wearers should consult the user manual provided by the pacemaker manufacturer or contact the pacemaker manufacturer to determine the effect on a specific pacemaker. Pacemaker wearers should also always notify their physician and discuss the health risks of being in proximity to magnetic fields. Wearers of metal prosthetics and implants should contact their physician to determine if a danger exists.

A table on the back of the *5-Gauss Warning Sign* shows the typical 5-gauss stray field for various magnet systems.

WARNING: **Keep metal objects outside the 10-gauss perimeter of the magnet.**

The strong magnetic field surrounding the magnet attracts objects containing steel, iron, or other ferromagnetic materials, which includes most ordinary tools, electronic equipment, compressed gas cylinders, steel chairs, and steel carts. Unless restrained, such objects can suddenly fly towards the magnet, causing possible personal injury and extensive damage to the probe, dewar, and superconducting solenoid. The greater the mass of the object, the more the magnet attracts the object.

Only nonferromagnetic materials—plastics, aluminum, wood, nonmagnetic stainless steel, etc.—should be used in the area around the magnet. If an object is stuck to the magnet surface and cannot easily be removed by hand, contact Varian service for assistance.

Warning Notices (*continued*)

A table on the back of the *10-Gauss Warning Sign* shows the typical 10-gauss stray field for various magnet systems.

WARNING: **Only qualified maintenance personnel shall remove equipment covers or make internal adjustments.**

Dangerous high voltages that can kill or injure exist inside the instrument. Before working inside a cabinet, turn off the main system power switch located on the back of the console.

WARNING: **Do not substitute parts or modify the instrument.**

Any unauthorized modification could injure personnel or damage equipment and potentially terminate the warranty agreements and/or service contract. Written authorization approved by a Varian Associates, Inc. product manager is required to implement any changes to the hardware of a Varian NMR spectrometer. Maintain safety features by referring system service to a Varian service office.

WARNING: **Do not operate in the presence of flammable gases or fumes.**

Operation with flammable gases or fumes present creates the risk of injury or death from toxic fumes, explosion, or fire.

WARNING: **Leave area immediately in the event of a magnet quench.**

If the magnet dewar should quench (sudden appearance of gasses from the top of the dewar), leave the area immediately. Sudden release of helium or nitrogen gases can rapidly displace oxygen in an enclosed space creating a possibility of asphyxiation. Do not return until the oxygen level returns to normal.

WARNING: **Avoid helium or nitrogen contact with any part of the body.**

In contact with the body, helium and nitrogen can cause an injury similar to a burn. Never place your head over the helium and nitrogen exit tubes on top of the magnet. If helium or nitrogen contacts the body, seek immediate medical attention, especially if the skin is blistered or the eyes are affected.

WARNING: **Do not look down the upper barrel.**

Unless the probe is removed from the magnet, never look down the upper barrel. You could be injured by the sample tube as it ejects pneumatically from the probe.

WARNING: **Do not exceed the boiling or freezing point of a sample during variable temperature experiments.**

A sample tube subjected to a change in temperature can build up excessive pressure, which can break the sample tube glass and cause injury by flying glass and toxic materials. To avoid this hazard, establish the freezing and boiling point of a sample before doing a variable temperature experiment.

Warning Notices (*continued*)

WARNING: **Support the magnet and prevent it from tipping over.**

The magnet dewar has a high center of gravity and could tip over in an earthquake or after being struck by a large object, injuring personnel and causing sudden, dangerous release of nitrogen and helium gasses from the dewar. Therefore, the magnet must be supported by at least one of two methods: with ropes suspended from the ceiling or with the antivibration legs bolted to the floor. Refer to the *Installation Planning Manual* for details.

WARNING: **Do not remove the relief valves on the vent tubes.**

The relief valves prevent air from entering the nitrogen and helium vent tubes. Air that enters the magnet contains moisture that can freeze, causing blockage of the vent tubes and possibly extensive damage to the magnet. It could also cause a sudden dangerous release of nitrogen and helium gases from the dewar. Except when transferring nitrogen or helium, be certain that the relief valves are secured on the vent tubes.

WARNING: **On magnets with removable quench tubes, keep the tubes in place except during helium servicing.**

On Varian 200- and 300-MHz 54-mm magnets only, the dewar includes removable helium vent tubes. If the magnet dewar should quench (sudden appearance of gases from the top of the dewar) and the vent tubes are not in place, the helium gas would be partially vented sideways, possibly injuring the skin and eyes of personnel beside the magnet. During helium servicing, when the tubes must be removed, follow carefully the instructions and safety precautions given in the manual *Varian Magnet Installation and Maintenance.*

Caution Notices

Observe the following precautions during installation, operation, maintenance, and repair of the instrument. Failure to comply with these cautions, or with specific cautions elsewhere in Varian manuals, violates safety standards of design, manufacture, and intended use of the instrument. Varian assumes no liability for customer failure to comply with these precautions.

CAUTION: **Keep magnetic media, ATM and credit cards, and watches outside the 5-gauss perimeter of the magnet.**

The strong magnetic field surrounding a superconducting magnet can erase magnetic media such as floppy disks and tapes. The field can also damage the strip of magnetic media found on credit cards, automatic teller machine (ATM) cards, and similar plastic cards. Many wrist and pocket watches are also susceptible to damage from intense magnetism.

A table on the back of the *5-Gauss Warning Sign* shows the typical 5-gauss stray field for various magnet systems.

Caution Notices (*continued*)

CAUTION: **Check helium and nitrogen gas flowmeters daily.**

Record the readings to establish the operating level. The readings will vary somewhat because of changes in barometric pressure from weather fronts. If the readings for either gas should change abruptly, contact qualified maintenance personnel. Failure to correct the cause of abnormal readings could result in extensive equipment damage.

CAUTION: **Never operate solids high-power amplifiers with liquids probes.**

On systems with solids high-power amplifiers, never operate the amplifiers with a liquids probe. The high power available from these amplifiers will destroy liquids probes. Use the appropriate high-power probe with the high-power amplifier.

CAUTION: **Take electrostatic discharge (ESD) precautions to avoid damage to sensitive electronic components.**

Wear grounded antistatic wristband or equivalent before touching any parts inside the doors and covers of the spectrometer system. Also, take ESD precautions when working near the exposed cable connectors on the back of the console.

Radio-Frequency Emission Regulations

The covers on the instrument form a barrier to radio-frequency (rf) energy. Removing any of the covers or modifying the instrument may lead to increased susceptibility to rf interference within the instrument and may increase the rf energy transmitted by the instrument in violation of regulations covering rf emissions. It is the operator's responsibility to maintain the instrument in a condition that does not violate rf emission requirements.

Introduction

This manual is designed to acquaint you with the basics of operating a Varian high-resolution NMR spectrometer system running VNMR 6.1B (VNMR is Varian's NMR application software package). The manual contains the following chapters:

- Chapter 1, "Overview of Varian NMR," introduces you to the Varian NMR system, its user interface, advanced features, and how VNMR and UNIX files are organized.
- Chapter 2, "VNMR Basics," covers entering and exiting VNMR and working with VNMR on the host computer.
- Chapter 3, "Using GLIDE," explains the basics of *GLIDE, a* user interface designed for walk-up NMR operation.
- Chapter 4, "Using the VNMR Menu System," covers using the buttons in the VNMR menu system, another user interface that simplifies NMR operation.
- Chapter 5, "Using the Command Mode," covers the basics of using the command mode to enter commands, macros, and parameter settings.
- Chapter 6, "Preparing for an Experiment," describes how to prepare for an NMR experiment, including preparing and inserting the sample, tuning the probe, spinning the sample, optimizing lock, and adjusting shims.
- Chapter 7, "Acquiring Data," covers setting parameters, using experiment text files, performing acquisition, and applying digital filtering.
- Chapter 8, "Data Processing," describes weighting functions, Fourier transformation, phasing, and advanced data processing.
- Chapter 9, "Display, Plotting, and Printing," covers FID and spectra display, plotting, integration, printing, and user-controllable line drawing.
- Chapter 10, "Storing, Retrieving, and Moving Data," explains working with directories, files, and data, including Ethernet, magnetic tape, and data compression.

The manual also contains a glossary covering common Varian NMR and VNMR terms.

Notational Conventions

The following notational conventions are used throughout all VNMR manuals:

- `Typewriter-like characters` identify VNMR and UNIX commands, parameters, directories, and file names in the text of the manual. For example: The `shutdown` command is in the `/etc` directory.
- `Typewriter-like characters` also show text displayed on the screen, including the text echoed on the screen as you enter commands. For example: `Self test completed successfully.`
- Text shown between angled brackets in a syntax entry is optional. For example, if the syntax is `seqgen s2pul<.c>`, entering the "`.c`" suffix is optional, and typing `seqgen s2pul.c` or `seqgen s2pul` is functionally the same.
- Lines of text containing command syntax, examples of statements, source code, and similar material are often too long to fit the width of the page. To show that a line of text had to be broken to fit into the manual, the line is cut at a convenient point (such

as at a comma near the right edge of the column), a backslash (\) is inserted at the cut, and the line is continued as the next line of text. This notation will be familiar to C programmers. Note that the backslash is not part of the line and, except for C source code, should not be typed when entering the line.

- Because pressing the Return key is required at the end of almost every command or line of text you type on the keyboard, use of the Return key will be mentioned only in cases where it is *not* used. This convention avoids repeating the instruction “press the Return key” throughout most of this manual.
- Text with a change bar (like this paragraph) identifies material new to VNMR 6.1B that was not in the previous version of VNMR. Refer to the *VNMR 6.1B Release Notes* for a description of new features to the software.

Other Manuals

This manual should help you get started in learning how to work with Varian NMR spectrometer systems and software. Other VNMR 6.1 manuals you should have include:

- *Walkup NMR Using GLIDE*
- *User Guide: Liquids NMR*
- *User Guide: Solid-State NMR*
- *User Guide: Imaging*
- *VNMR Command and Parameter Reference*
- *VNMR User Programming*
- *VNMR and Solaris Software Installation*

All of these manuals are shipped with the VNMR software. These manuals, other Varian hardware and installation manuals, and most Varian accessory manuals are also provided online so that you can view the pages on your workstation and print copies.

Types of Varian Spectrometer Systems

In parts of this manual, the type of system—UNITY*INOVA*, *MERCURY* VxWorks Powered (shortened to *MERCURY-VX* throughout all manuals), *MERCURY*, *GEMINI 2000*, UNITY*plus*, UNITY, or VXR-S—must be considered in order to use the software properly.

- UNITY*INOVA* and *MERCURY-VX* are the current systems sold by Varian.
- UNITY*plus*, UNITY, and VXR-S are spectrometer lines that preceded the UNITY*INOVA*.
- *MERCURY* and *GEMINI 2000* are a separate line of spectrometers that preceded the *MERCURY-VX*.

Chapter 1. Overview of Varian NMR

Sections in this chapter:

- 1.1 “Varian NMR Spectrometer System” this page
- 1.2 “User Interface” page 25
- 1.3 “Advanced Features” page 29
- 1.4 “Introduction to UNIX and VNMR Files” page 33

1.1 Varian NMR Spectrometer System

The Varian research NMR spectrometer system consists of four major units:

- *Host computer* – A workstation that controls the spectrometer, thus receiving most of your attention in day-to-day use. As such, it takes the major share of the attention in this manual.
- *NMR system console* – The main unit of the spectrometer system. Housed in one, two, three, or four cabinets, depending on the model and configuration of the spectrometer, the system console contains digital and rf (radio-frequency) circuit boards, amplifiers, frequency synthesizers, power supplies, and other assemblies. With the exception of an occasional special experiment that requires reconfiguring some of the acquisition hardware, you will rarely need to even open a console door.
- *Superconducting magnet* – The magnet holds the probe and provides a stable magnetic field. Units enclosed or attached to the magnet leg, or standing on the floor beside the magnet, contain rf control circuitry and amplifiers as well as air control systems for spinning, cooling, and lifting the sample.
- *Probe* – The probe transmits rf power to the sample and detects minute voltages in return. Many sizes and types of probes are available, including broadband and switchable probes that allow observing most nuclei of relevance without changing the probe. Routine sample-to-sample probe tuning is covered in Chapter 6, “Preparing for an Experiment,” while changing probes and tuning the probe to other nuclei is discussed in the installation manual for the probe.

Host Computer

The host computer, based on a Sun Microsystems workstation, controls the spectrometer. The primary user interaction with the host computer occurs through the display screen, three-button mouse, and keyboard. The use of these devices is introduced in the section “User Interface” on page 25.

A wide range of Sun desktop workstations can be used with a system. The standard workstation contains a hard-disk drive to store data and a magnetic tape unit for saving and transferring data. If additional data storage is necessary, a second hard-disk drive can be

added to the system. A CD-ROM drive must also be available, either local or on a network, for installing the current versions of Sun and Varian software. System printers, plotters, additional memory, and other computer peripherals can be added to the basic system.

NMR System Console

The NMR system console contains rf electronics, including transmitters, amplifiers, and receivers, as well as a complete computer system known as the *acquisition computer*. Units in the acquisition computer control the pulses and timing of the acquisition process (through the Digital Acquisition Controller board, Pulse Sequence Controller board, Acquisition Controller board, or Output board, depending on the system), digitize the signal (through the analog-to-digital converter or ADC), and automatically sum the data and scale it when necessary (the $^{1}H/^{13}C$ *GEMINI 2000* uses software data summing). The acquisition computer is also responsible for the control of the spinner and magnet homogeneity.

Each of the console units is controlled by the main processor, which contains pulse sequence control information programmed in its memory. The type of communication between the host computer and the acquisition computer is system-dependent:

- UNITY*INOVA* and *MERCURY-VX* systems use Ethernet, with control by an integrated chip on the acquisition computer board.
- *MERCURY* and *GEMINI 2000* systems also use Ethernet, but control is by a Ethernet board.
- UNITY*plus* and UNITY systems use a SCSI high-speed link through a second computer in the acquisition unit, known as Host-Acquisition Link, or HAL. This computer provides a 2-MB memory into which data acquisition is performed.

Implementing the pulse sequence involves timing certain operations of the transmitter, decoupler, and receiver. The transmitter produces a radio frequency at the frequency selected (the parameter `sfrq`) for the nucleus being observed. In another section of the rf electronics, another frequency (in most instruments, this is the proton frequency) is sent to the decoupler. In order to maintain long-term electronic stability, the instrument also generates a lock frequency that is normally set at the deuterium frequency. A deuterated solvent is used in most cases (although the spectrometer can be operated unlocked) so that the deuterium rf can be locked onto the deuterium resonance of the solvent.

Up to eight rf channels are available on UNITY*INOVA* systems. *MERCURY-VX*, *MERCURY*, and *GEMINI 2000* systems have two channels. The main features of additional channels on UNITY*INOVA* include independently generated rf, high-speed line control of the rf transmitter board, a dedicated linear pulse amplifier, and channel independence—each channel is separate.

A waveform accessory can be also be integrated into the UNITY*INOVA* console, with as many as four waveform generators. This option is not available on the *MERCURY-VX*, *MERCURY*, and *GEMINI 2000* systems.

Varian features a wide range of gradient and shim systems in many sample sizes and for all applications—liquids, solids, and imaging. For pulsed field gradient (PFG) experiments, your system may have one of the Performa PFG modules. Varian shim systems range from 13 channels for the *GEMINI 2000* and UNITY and VXRS systems to 40 channels for the Ultra•nmr shim system II. *MERCURY-VX* and *MERCURY* are 14 channels.

Superconducting Magnet and Probe

The superconducting magnet and probe, although separate, are closely related. The types and configuration of these components and associated electronics differ between systems. Figure 1 shows two representative systems.

On systems without sample changers, the user's primary interaction with the magnet and probe is to insert the sample into the hole at the top of the magnet. Under some circumstances, the probe needs to be tuned to electronically match the sample and experiment desired. For this purpose (depending on the type of probe), there may be tuning rods extending from the probe, a tuning meter, a tuning selector switch that chooses between tuning the observe and decouple channels of the probe, and a tuning gain knob that controls the sensitivity of the tune signal used for tuning a channel.

- On UNITY*INOVA* and UNITY*plus* systems, a digital display on the TUNE INTERFACE unit, attached to the magnet leg or to the dual preamplifier, shows reflected power. Dual push-button switches below the digital display activate the tuning circuit, select the channel, and set the sensitivity of the channel during the tune operation.
- On *MERCURY-VX*, *MERCURY*, and *GEMINI 2000* systems, reflective power is shown in a "needle micrometer" indicator on the magnet leg. An adjacent toggle switch on the magnet leg selects whether the meter displays reflective power for tuning or the spinning rate. For normal operation, the switch is set for the spin rate. UNITY and VXR-S systems use a similar display to the *MERCURY*.

Chapter 6, "Preparing for an Experiment," describes probe tuning procedures. For details about installing and tuning probes, refer to the probe manual shipped with the probe.

1.2 User Interface

The host computer for the spectrometer includes a number of highly advanced concepts, including multiple experiment capability, multitasking, windowing, and automatic queuing. The system, however, was designed with the user in mind, so it is easy to operate. This section briefly describes how you interacts with the data system through three devices: the mouse, the keyboard, and the display monitor. Chapter 2, "VNMR Basics," contains a detailed description of the user interface and VNMR display.

VNMR Software

The host computer for the spectrometer is a Sun Microsystems workstation that runs the Varian NMR software program, called VNMR. The VNMR software package supports data acquisition, processing, display, and data analysis for the entire range of applications—liquids, pulsed field gradients, solids, and imaging.

VNMR is available in three versions:

- The VnmrX version is used if the Sun is running OpenWindows™ or the Common Desktop Environment (CDE) windowing environment (both are based on the X Window System). This version allows remote operation from other workstations, X terminals, or personal computers such as a PC or a Macintosh. Spectrometer status can be monitored, data processed during acquisition, shims adjusted, and new experiments queued from a remote location.
- The VnmrI version is available for workstations from IBM, and the VnmrSGI version is intended for Silicon Graphics workstations. VnmrI and VnmrSGI have essentially the same user capabilities, look, and feel of the VnmrX version.

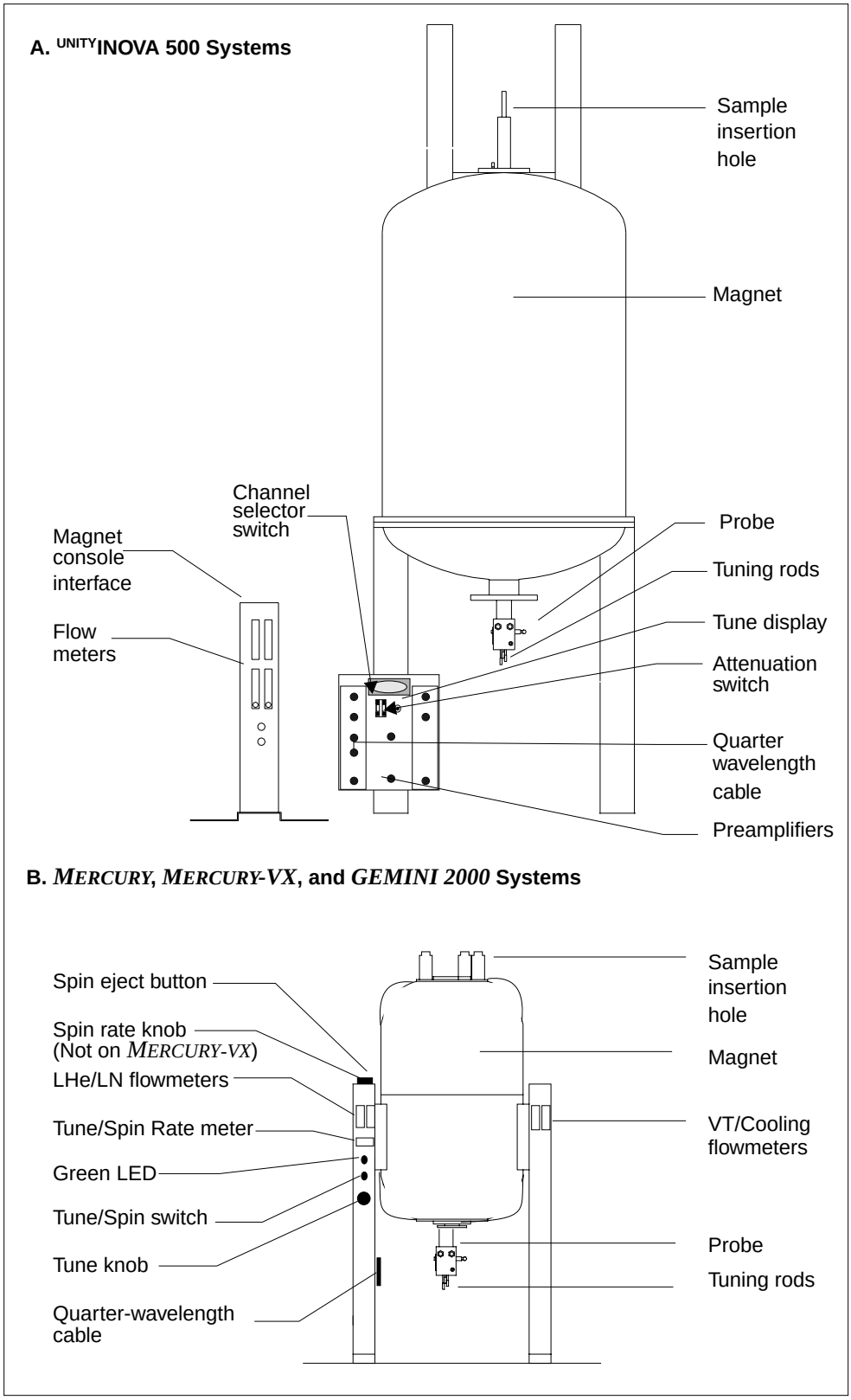

Figure 1. Magnet, Probe, and Associated Electronics

Mouse, Keyboard, and Remote Status Module

The mouse is a three-button pointing device that controls one or more cursors that appear on the display screen (although only one cursor can be controlled at a time).

On the keyboard, you enter commands, parameters, and other alphanumeric information into the data system.

The optional remote status module is a small case containing indicators and displays, usually placed next to the host computer display. The UNITY*INOVA* and UNITY*plus* versions of the module display such information as the status and temperature of the variable temperature unit, lock level, acquisition, and other information for each active rf channel. *MERCURY-VX*, *MERCURY*, and *GEMINI 2000* systems use an indicator on the magnet leg.

VNMR Display Screen

The VNMR display screen shows you what is happening with the data. Figure 2 shows a typical configuration of this screen.

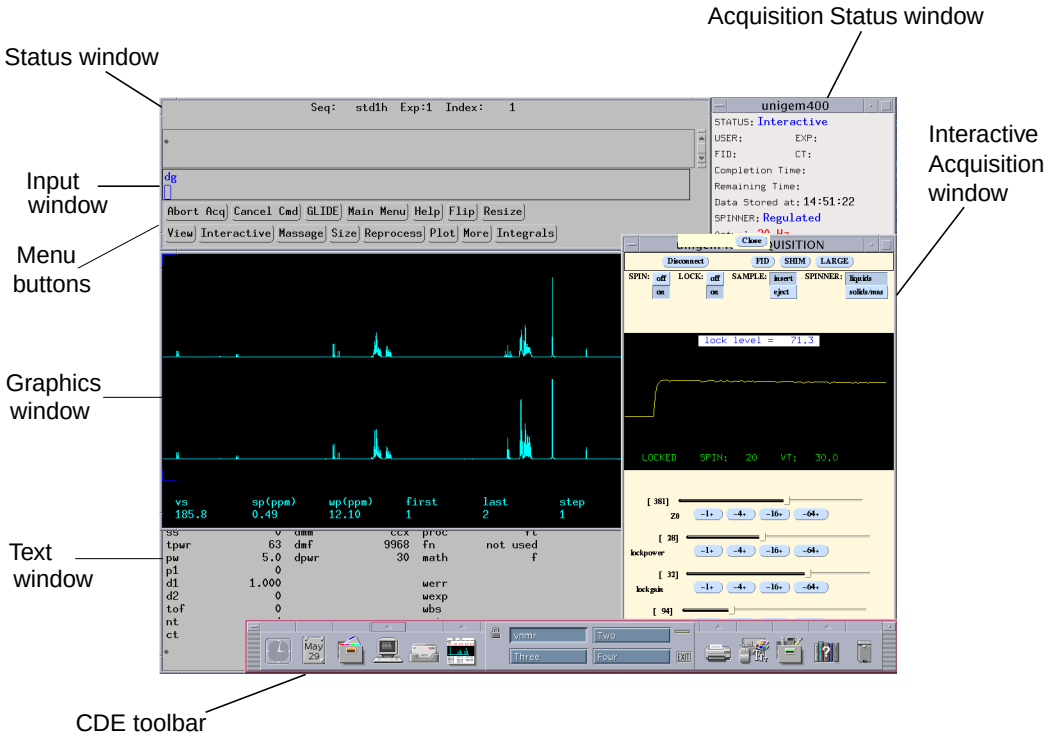

Figure 2. VNMR Display Screen

The display is divided into several windows. The menu buttons, graphics window, and text window are typically always visible. Like most windowing systems, these windows can be moved, resized, and even closed.

The windows are described here, and throughout the manual, according to their standard positions.

On the VnmrX version of VNMR, the *GLIDE* user interface (see Figure 3) is typically at the top of the screen.

Figure 3. *GLIDE* User Interface

If the system is configured to perform acquisition, not as a stand-alone data station, the right side of the screen often displays two other windows—the Acquisition Status window and the Acquisition window. Both windows are shown in Figure 2.

If the system is running the Common Desktop Environment (CDE), the CDE toolbar, which includes a custom tool to activate VNMR, shown in Figure 4 is displayed on the bottom of the screen.

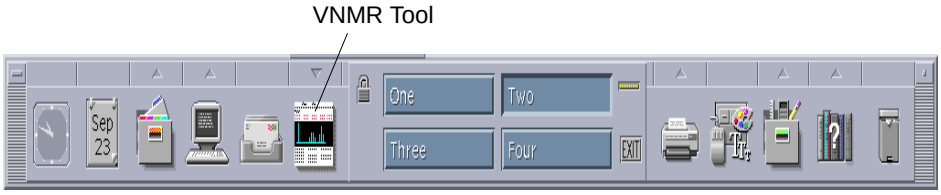

Figure 4. CDE Toolbar

The part of the screen where no windows appear is called the *workspace*. On a typical system, the workspace contains artwork or a repeating design. The default design is the Varian logo and name repeated in a grid over the background, but the workspace can be customized locally.

Other objects that usually appear on the VNMR display screen include icons for closed windows. Typically, such icons for the console and VNMR appear on the opening screen.

Using Multiple Windows

You can configure the graphics window into smaller panes, dividing it into one, two, or three distinct graphical rows and/or columns. Each pane can be used independently of others.

Activating Window Panes

After you create multiple window panes, only one pane can be worked on at a time. You can activate other panes by double-clicking in them with the left mouse button. If two panes represent two separate experiments, double-clicking in either pane automatically joins the appropriate experiment. Whatever activity was running in the panes is remembered and restarted.

Creating Multiple Windows

To create multiple windows, do the following procedure:

1. Click **Main Menu**, **More**, **Windows**. The windows menu opens, as shown in Figure 5.

Figure 5. Windows Menu

2. Select the number of rows and columns of panes that you want to appear in the graphics window.

Selecting Fonts

To select fonts for each window, do the following procedure:

1. Click **Main Menu** > **More** > **Windows**.
2. Click on the **Select Fonts** button to open the FontSelect window, shown in Figure 6.

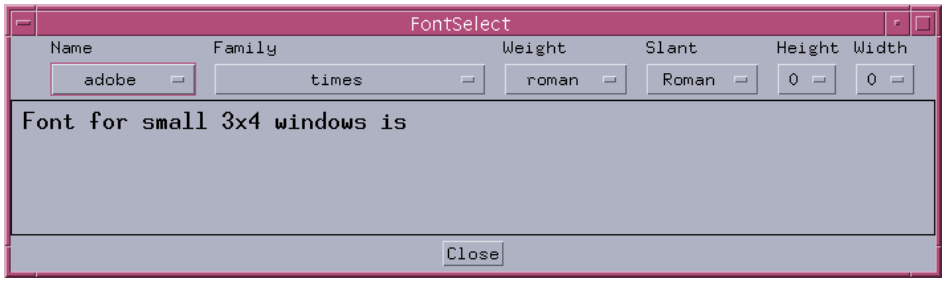

Figure 6. FontSelect Window

3. Click on the corresponding buttons to choose the font **Name**, **Family**, **Weight**, **Slant**, **Height**, and **Width**. Exit the window by clicking **Close**.

Multiple Window Commands

The multiple window environment is controlled by the following commands:

- `setgrid` sets the number of rows and columns in the graphics windows.
- `fontselect` opens the FontSelect window that enables you to define fonts for the panes.
- `jwin` is called at each double-click of the left mouse button inside a pane. This macro records the activity in a current window and then restarts the activity in the selected window, including a `jexp` command if necessary. `jwin` calls `setwin` to activate the selected window. The global parameters `curwin` and `mapwin` maintain information about the panes.

1.3 Advanced Features

The data system incorporates many advanced operating features, including queuing, multitasking, multi-FID experiments, multidata sets, MAGICAL II macro language, and optional specialized software.

Queuing

Virtually all operations on the data system are *queued*, that is, you are free to ask the system to perform any action at any time, even in circumstances in which that action cannot possibly occur immediately. For example, suppose you give the system a command to plot a spectrum and that plot starts. You do not need to wait for that plot to finish, but instead can proceed to set up a second plot and issue the command to perform that plot as well. Because the first plot is still occurring, the system queues up your request and performs it when the resources needed to perform the task (in this case, the plotter) are free. As far as you are concerned, the plot is now "done," and you can move on to the next task.

Another important example of queuing on the system occurs with data acquisition. Just like plotting, you need not be concerned whether an acquisition is in progress when you set up an experiment and issue the command to start the acquisition. If no acquisition is in progress at that time, any acquisition you request starts immediately. If an acquisition is in progress, your acquisition request waits until the current acquisition is finished, and starts at that time. Because a particular acquisition can take many hours, the system even enhances the queuing feature by informing you of the projected completion time of the current acquisition, so you will know when the next one begins.

Note that queuing is fully automatic and requires no special commands or other operations.

Multitasking

Unlike queuing, which occurs sequentially, the multitasking feature of the system allows simultaneous activities to occur. The data system includes a number of computers and microprocessors, all of which can be active at the same time. On UNITY*INOVA* systems, the acquisition computer's operating system is multitasking, which allows data acquisition, data transfer, and status checking simultaneously. In addition, the UNIX operating system used on the host computer allows multiple tasks, such as printing, plotting, data processing, and communication with other computers, to all proceed at the same time, even with a single processor.

Multitasking is like queuing in one respect—you do not have to do or know anything special. Issuing successive commands to initiate an acquisition, a plot, some printing, and some data processing quickly causes four processes to become active simultaneously. Just like queuing, the rule is simple—tell the system what you want to do whenever you wish. If the operation you request requires queuing, it is e queued. If it can be accomplished immediately and involves multitasking, that happens as well.

Multitasking has one limitation, however. In normal circumstances, the system is not designed to perform multiple data processing operations simultaneously *within a single copy of the VNMR software*. Thus, while it is possible to have two or more terminals attached to a computer and several users performing a 2D transformation at the same time, it is not possible for a single user to do multiple data processing tasks from a single terminal.

Concurrent processing operations are possible outside the VNMR program by using UNIX. For example, assume you have started a long 2D Fourier transformation (FT) in the VNMR program. You are now free to open (or re-open) a different window, which puts you in communication with the UNIX operating system or with one of the many programs supplied with UNIX (text editors, compilers, etc.). Thus, you can edit a new pulse sequence or write a report on your most recent results while the Fourier transform proceeds.

It is even possible to start another copy of VNMR running in a noninteractive background mode. If you had an extremely long operation to perform, such as an 8K x 8K 2D Fourier transform, this operation could be performed in this background mode, leaving your

interactive copy of VNMR free to start the next acquisition or do some spectral display and plotting, etc. More information on the background mode of VNMR is found in the manual *VNMR User Programming*.

Within the NMR software package, there is also an important part of the software that is separate from the basic VNMR program, and that is the Acquisition window. This window permits locking and shimming, FID display, and interactive parameter adjustment (IPA). Because this activity runs in a separate window, it is a permissible multitasking activity. Thus, even while a long transform is occurring, you can insert the next sample and start performing locking and shimming.

Experiments

NMR scientists, like all scientists, are accustomed to performing experiments. For this reason, the data system organizes its data along the same lines. In VNMR, an *experiment* is a directory, on a disk, in which parameters and data are stored. The values of the parameters represent the conditions under which the data in the file was collected or will be collected. Each experiment has a number (shown by "`Exp:`" on the first line of the status window), which can be 1, 2, on up to 9999. We refer to these experiments as `exp1`, `exp2`, `exp3`, and so on. Different experiments can hold different sets of data.

The `explib` program gives a view of the experiments on a system by displaying a list of the experiments that exist, their size, and information about the current data contained in that experiment.

An experiment has room, simultaneously, for both the raw data (the FID) and the processed data (the transformed spectrum). Thus, it is not necessary to remember to "save the data" before performing an FT or other processing; the original data is always unaffected. Each experiment always contains some data, namely the last data that was collected in that experiment (just like parameters always contain the last value that was entered). Data remains in an experiment until you return to that experiment and begins a new acquisition. Thus, an experiment is basically the mechanism for temporary data storage—a place for the data while it is being acquired, processed, or plotted. When done with the data, it should be saved in a permanent file, freeing the experiment for another set of data.

Multiple Related FIDs

Many experiments require obtaining a series of FIDs related to each other through the variation of one or more parameters. For example, suppose it is necessary to run a series of spectra at four different temperatures: 30°C, 50°C, 70°C, and 90°C. Instead of acquiring four separate sets of data, it is possible to create an *array* in which the `temp` parameter is given four successively different values:

```
temp=30,50,70,90.
```

These four subexperiments are now all treated as a single experiment. One `go` command successively begins acquisition of all four subexperiments. One command can be used to transform all the spectra, one command to display all the spectra on the screen simultaneously, one command to plot all the spectra, and one command to save all the spectra. Virtually all of the parameters affecting acquisition can be arrayed in this way, making for a simple and convenient method of performing pulse width calibrations, optimizing parameters, etc.

Multiple Unrelated Sets of Data

Sometimes it becomes desirable to deal with multiple sets of data that are *not* related to each other simply by arraying some parameter. For example, you may want to obtain a carbon and a proton spectrum on the same sample, where the parameters and the data are completely different. You may want to obtain spectra with the same parameters, but on different samples.

Of course, it is perfectly possible to acquire one such data set, process it, plot it, save it on disk, acquire the next data, process, plot, save, and so on. But this procedure results in an inefficient use of the system. In acquiring one spectrum, for example, it would be more efficient to start a second acquisition (another nucleus, another pulse sequence, another sample), and then process the first while the second is being acquired. Of course, this routine can be extended to more than two data sets, in fact, up to nine.

To simultaneously work with two different sets of data (such as processing one set and acquiring another), you use two (or more) experiments. For example, first enter `go` to acquire data in `exp1`. Next, join `exp2` by entering `jexp2` and starting another experiment. Then enter `jexp1` to rejoin `exp1` and process and plot the first spectrum (`exp1`) while the second (`exp2`) is being acquired.

To follow the second experiment with a third (even though the second is still being acquired), join `exp3` by entering `jexp3`, select parameters, and start another experiment. Since an acquisition is in progress, this experiment (`exp3`) is queued up behind the second, just as for other forms of queuing previously discussed. Now you can go back to `exp1`, process more, then enter `jexp2` to look at that data, either when it finishes or before, and so on. If the `text` command is used to annotate sufficiently each experiment, the `explib` command enables us to juggle all these functions with ease.

MAGICAL II Macro Language

A *macro* is a single command that duplicates any series of commands and parameters enterable on the keyboard. Routinely used in daily operation, a macro is not a necessary function of the system, but is extremely useful.

Suppose every time a spectrum is plotted, it is desired to have parameters printed, a scale plotted below the spectrum, and peaks above 20 mm in height labeled as to frequency. This can be done by typing

```
pl pscale pap page th=20 printon dll printoff
```

which is not too difficult if the spectrum is plotted once, but what if a similar spectrum must be plotted 5 times or 500 times?

The answer is to create a macro command that executes the exact series of the listed commands and parameters. The name of the macro can be any convenient name, such as `plc13`, or `plc`, or just `c`. Whatever the name chosen by the user, the system uses that name exactly like any other system command.

Macros are extensively used to set up the various special pulse sequence experiments that are available. Thus, if a conventional ^{13}C spectrum has been acquired, entering `apt` executes the macro `apt` that sets up an APT experiment. Or, starting with a conventional ^{1}H spectrum and typing `cosy` sets up a 2D COSY experiment. Macro commands can simplify the most complex set of commands and parameters.

Macros on the system are written in a macro language called MAGICAL™ II (for MAGnetics Instrument Control and Analysis Language II) that is built into VNMR. MAGICAL is an extremely powerful language that combines three essential elements:

- Programming language features, like conditional statements.
- Direct access to key features of the NMR data, such as peak heights, integrals, and frequencies.
- NMR parameters treated as variables in a computer program.

Unlike MAGICAL (the predecessor to MAGICAL II), which operated relatively slowly using an interpreted mode, MAGICAL II macros are parsed so that their execution is extremely rapid. Indeed, many of the standard commands in the VNMR software are written in MAGICAL II, and yet they run essentially at the same speed they would have run if they had been written in a more traditional language such as C.

Besides allowing creation of customized NMR algorithms for data acquisition or analysis, MAGICAL II also allows data acquisition and analysis to be linked for adaptive acquisition, a critical capability for applications such as the LC-NMR.

One of the interesting attributes of MAGICAL II is that all of its features can be directly executed from the keyboard without actually creating a macro. Do you want to double the vertical scale? Just enter

```
vs=vs*2
```

Do you want to display the central 50% of the spectrum? Simply enter

```
f wp=0.5*sw sp=sp+wp/2
```

You can even write a simple computer program directly from the keyboard. Would you like to compute 2^7? Try entering the following and see if you get the right answer:

```
r1=1 r2=1 repeat r1=2*r1 r2=r2+1 until r2>7 r1?
```

MAGICAL II is discussed in detail in the manual *VNMR User Programming*. Users who wish to modify the existing software or add their own macros are strongly encouraged to learn to use MAGICAL II.

Optional Specialized Software

Much advanced, specialized software is available for VNMR, including the following optional packages sold by Varian:

- Bayes software uses Bayesian probability theory to directly analyze 1D, time-domain data, providing signal amplitude, frequency, and linewidth for all statistically significant resonances.
- Diffusion software performs acquisition and analysis for the determination of diffusion constants using the pulse gradient echo method.
- FRED™ software discovers carbon connectivities at previously unattainable levels of sensitivity. FRED analyzes data from the insensitive but powerful carbon-carbon connectivity experiment.
- STARS™ software simulates single-pulse experiments on solids.

1.4 Introduction to UNIX and VNMR Files

The current VNMR software package runs in the *Solaris* 2.*x* computing environment, which includes SunOS 5.x (Sun's implementation of UNIX), the OpenWindows and CDE windowing environments, and desktop tools such as Clock and File Manager.

No attempt is made in this manual to teach you more than is necessary about Solaris, OpenWindows, CDE, and UNIX except for you to run VNMR. Sun provides extensive information about their products, both online and hard copy.

UNIX File System

Like any high-level system, data on your disk is found in files, which are themselves organized into directories. The UNIX file system is traditionally depicted in a tree structure, with all files and directories are hierarchically organized into a top-level directory whose symbol is a slash (`/`) and name is `root`. The `root` directory ultimately contains all other directories and files.

VNMR Directories and Files

Figure 7 is a diagram of the part of the UNIX file system that is important in using VNMR software. In the diagram, the directories `vnmr`, `home`, and `usr` are shown as subdirectories of `root` (`/`). To identify these directories as first-level subdirectories of `root`, a slash is placed in front of the directory name: `/vnmr`, `/export/home`, and `/usr`.

Knowing the location and contents of system directories and files used by VNMR is helpful when trying to understand the UNIX file system:

`/vnmr`	Contains all VNMR software (on Solaris, `/vnmr` is actually a link to `/export/home/vnmr`, so `vnmr` is also in the directory `home`.
`/export/home`	Contains the default location for users' home directories.
`/usr`	Contains UNIX libraries and online reference materials.

The `/vnmr` directory contains numerous subdirectories, including:

`acqbin`	Contains commands related to the data acquisition process.
`acrobat`	Contains files and reader software for *VNMR Online*.
`bin`	Contains commands used for VNMR but executed from UNIX.
`fidlib`	Contains directories with FID data and parameter files that can be used to practice data processing if no spectrometer is available to generate real data. Many of the examples used in this manual guide you through a step-by-step approach to one or another aspect of using the software, based on the data in this directory.
`glide`	Contains the files used by the *GLIDE* user interface.
`help`	Contains help files for the VNMR menu system.
`kermit`	Contains the public domain serial communications program `kermit` and the related help file `kermit.doc`.
`lib`	Contains software libraries, each a collection of routines, used by VNMR and PSG.
`maclib`	Contains numerous text files for system macros written in the MAGICAL II language. The files can be modified by the system administrator (described in "NMR System Administrator and Other Users" on page 36) if desired.
`manual`	Contains text files providing help in using VNMR commands.
`menulib`	Contains numerous system menus written in the MAGICAL II language. The system administrator can modify these menus.
`nuctables`	Contains text files for looking up a nucleus and translating it into the appropriate transmitter and decoupler frequencies for the rf type and field strength in use.

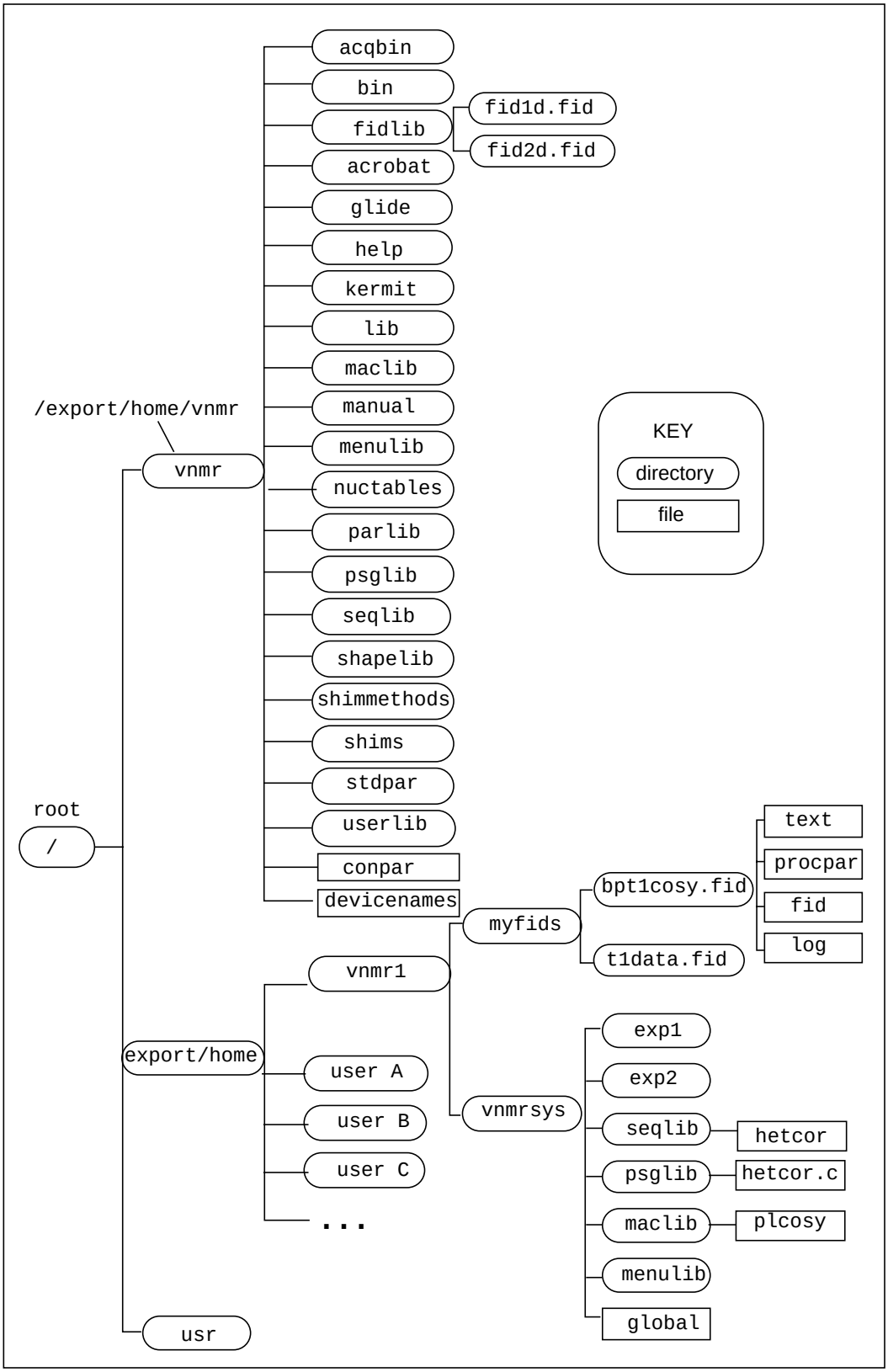

Figure 7. File Structure Overview

`parlib`	Contains files that store one parameter set for each pulse sequence, so that parameters or parameter values unique to that experiment can be recalled from that file.
`psg`	Contains source code for pulse sequence statements.
`psglib`	Contains files holding the source code listings of the pulse sequences supplied with the system. These files are *not* executable pulse sequences and must first be compiled to create a corresponding file in the `seqlib` directory.
`seqlib`	Contains compiled pulse sequences ready to be run on the system. A pulse sequence must be defined by a `seqlib` file in order to be run.
`shapelib`	Contains pulse shape definitions used by the pulse sequence generation (PSG) software.
`shimmethods`	Contains files with shim methods by which autoshimming is performed. A number of standard methods are supplied (see "Adjusting Shims" on page 135), but these can be augmented, so that algorithms of your own choosing can be used.
`shims`	Contains sets of shim settings. Each set might correspond to a particular probe or solvent, or perhaps just to a particular date.
`stdpar`	Contains a series of files, each named after a nucleus, that contain the standard parameter sets for that nucleus.
`userlib`	Contains user-contributed files similar to the system files found in the `/vnmr` directory: `maclib`, `psglib`, `menulib`, etc.

Besides these directories, at least two files in the `/vnmr` directory are of interest:

`conpar`	When the system is first installed, or when changes are made, the configuration parameter file `conpar` is modified to reflect the changes. These parameters, such as the spectrometer frequency, are common to all users and hence placed in a system file.
`devicenames`	A file listing possible choices for printers and plotter and identifying which of these devices are attached to your computer (or to other Sun computers networked together via Ethernet).

NMR System Administrator and Other Users

The `/export/home` directory contains one directory for each user who has been given permission to use the system (user A, user B, etc. in Figure 4). Every system is initialized with a special user named `vnmr1`, who is the NMR system administrator, the "owner" of the VNMR software (there is also a UNIX system administrator known by the standardized name `root`). Thus, `vnmr1` is the only user with permission to change the files found in the `/vnmr` directory.

In addition to being the NMR system administrator, `vnmr1` is also a regular user of VNMR, with permission to run NMR experiments, process data, etc. This capability is provided by the directory `vnmrsys`, which is found within the `vnmr1` directory (and whose full name, in UNIX terminology, is `/export/home/vnmr1/vnmrsys`).

The `vnmrsys` directory contains a series of essential files. One or more experiment files (`exp1`, `exp2`, etc.) are used to provide temporary homes for NMR data being acquired or processed; these files were previously discussed. Several directories that also existed in the `/vnmr` directory are found repeated here: `seqlib`, `psglib`, `maclib`, `menulib`, and `shims`. These directories are used to provide *user-specific* pulse sequences, macros, menus, and shim values.

Thus, a user who wishes to develop a personal version of the `plcosy` macro, which plots a COSY spectrum, is free to do so without affecting the software that can be "seen" by other

users. A user who wishes to modify the heteronuclear chemical shift correlation pulse sequence `hetcor` can similarly do so without affecting other users. Once the new version is proven to be more desirable, the NMR system administrator `vnmr1` can copy it into the directory `/vnmr/seqlib`, where it is accessible to all users.

Finally, a file named `global` is found in each user's directory. This file contains parameters that are common to all of a user's experiments, and that do not need to be repeated. For example, while a user may want to process proton spectra in `exp1` and carbon spectra in `exp2`, that user probably wants to plot them both on the same plotter, so the parameter `plotter` is found in `global` and not within `exp1` or `exp2`.

Many users operate their system with just one or two operators and might want to operate solely as `vnmr1` without concerning themselves with creating additional files for additional operators. In this case, we recommend leaving the `/vnmr` files to hold the software provided by Varian (pulse sequences, macros, etc.), while you put your own modifications into the `/export/home/vnmr1/vnmrsys` files.

Other system administrators might want to set up a system in which each operator or group has an individual directory. This can result in, for example, a series of files organized in a directory such as `/export/home/george` (where `george` could be `userA` in Figure 7), which contain the same series of files as found in `/export/home/vnmr1`.

The obvious question is, where should data be stored? You can create a directory at almost any location in this tree structure, in which you can subsequently store data in a permanent fashion (or at least before you transfer it to tape). A logical place, however, is within the user's subdirectory. Another alternative is to store data in a directory called `data` within `/export/home/username/vnmrsys/`. In Figure 7, for example, the directory `myfids` has been created within the home directory of user `vnmr1` and has been used to store two different FIDs.

A FID is not a single file but a directory with the following files:

- `fid` contains the raw data for the FID (a binary file).
- `procpar` contains parameters used to acquire and process the data (a text file).
- `text` describes the sample or experiment (a text file with your annotations).
- `log` contains the acquisition log (a text file).

FIDs have certain implications because directories are not copied or otherwise manipulated by UNIX in the same way as simple files, but require special commands.

Paths and the Working Directory

In UNIX, the *path* for a file or directory is a list of directories that lie between the top level of a file system (the `root` directory) and the file or directory. To build a path, list the successive directory names in order, starting with "`/`" (the symbol for the `root` directory), with each subdirectory separated by a "`/`", and the name of the file or directory as the last entry. For example, the path to the `global` file in the lower right of Figure 7, is `/export/home/vnmr1/vnmrsys/global`. Naming a file or directory this way is called an *absolute path* because every file and directory has a single, unique path.

To avoid the need to type in a long path to reach a file, UNIX provides the concept of the *working directory*. The working directory is the current directory you are "in." To show the name of this directory at any time, enter the UNIX command `pwd` (print working directory) and the absolute path is displayed. To change to another directory, enter the command `cd` (change directory) with the path of the directory you want to be in.

For example, if you enter `cd('/export/home/vnmr1/vnmrsys')` within VNMR, the directory `vnmrsys` becomes the new working directory. Since `global` is a file in the directory `/export/home/vnmr1/vnmrsys`, you can now refer to it by just `global` (e.g., `cd global`) rather than by the `/export/home/vnmr1/vnmrsys/global` absolute path. `global` is a relative path because it is a name relative to your current working directory. Notice that although the relative path is almost always shorter, to use a relative path you must know the name of the related working directory.

User Library

The Varian NMR user group library, placed in the `userlib` directory, contains a series of files similar to those found in the directory `/vnmr`: `maclib`, `psglib`, `menulib`, etc. The purpose of the user library is to provide a mechanism for user contributions in the area of pulse sequences, macros, menus, stand-alone programs, etc.

User contributions are briefly tested and checked for conformance to documentation standards, but are not "Varian software." The contributions are supported by online documentation, but not by Varian applications or service support personnel. Contributors can include the contributor's phone number, e-mail, FAX number, or address if they are willing to answer questions, but they are not obligated to do so.

The file `userlib/CONTENTS` provides an alphabetical listing of all files in these directories, together with a brief (one sentence or less) description of the file. More complete documentation for each file is found in the relevant directory, in a file by the same name as the file but with "`.README`" appended. The `README` file tells you who submitted the file, gives you a general overview of its purpose, and identifies its limitations (e.g., the file only works on a three rf channel system or requires linear amplifiers). Finally, files that provide new functionality to VNMR (some just modify or improve existing macros, pulse sequences, etc.) have an associated file in the `userlib/manual` directory with complete instructions on how to use this pulse sequence, macro, etc.

Complete instructions for using the material in the user library, and for submitting material to the library, are found in the `userlib/README` file. Users are encouraged to add to the value of the user library concept by contributing material to it, subject only to the requirement about providing online documentation to accompany the submitted material. The CD-ROM containing VNMR also contains a current copy of the Varian NMR user library. Refer to the manual *VNMR and Solaris Software Installation* for installation.

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Chapter 2. VNMR Basics

Sections in this chapter:

- 2.1 “Entering and Exiting VNMR” this page
- 2.2 “Working with VNMR on the Host Computer” page 41

You will find that you can work in VNMR through three different modes:

- *GLIDE* user interface
- VNMR menu system
- Command mode

These modes are generally interchangeable. You can use whichever mode you want, or even mix modes, to accomplish your goals. At times, you will also use certain UNIX commands outside the VNMR programs for certain NMR tasks.

2.1 Entering and Exiting VNMR

In some cases, the VNMR program is left running on the host computer at all times, and when you walk up to the workstation you just sit down and start using the system. In other cases, however, you may wish to take advantage of the login and logout features of UNIX, so you need to know how to enter and exit VNMR. The system administrator must understand this process, of course. Table 1 lists the commands and menu buttons associated with entering and exiting VNMR.

Table 1. Entering and Exiting VNMR

Command	
`acqi`	Open the Acquisition window
`acqstat<(remote_system)>`	Open the Acquisition Status window
`login` *`username`*	Log into UNIX with user name given (UNIX)
`logout`	Log out of UNIX (UNIX)
`exit`	Call the `vnmrexit` command
`vnmrexit`	Exit from VNMR system
Menu System	
Main Menu | More | Exit VNMR	Exit from VNMR system
Exit button on CDE toolbar	Exit from VNMR system

To Start VNMR

Before logging into the system, you must have a user name (shown by *`username`* in the following procedure) assigned by your system administrator. The standard software is installed so that `vnmr1` is always configured as a user, but your system administrator probably defined others as well.

1. If using the CDE interface, enter your user name in the login window.

   Otherwise, if a `login` prompt is displayed, enter your VNMR user name (remember to terminate your input by pressing the Return key):
   `login:` *`username`*

   If another prompt is displayed instead of the `login` prompt, enter the command `login` followed by your user name (e.g., `login vnmr1`).

2. If you are using the CDE interface, enter your password in the password window and press the Return key. Otherwise, if a `password` prompt is displayed, enter your password:
   `Password:` *`userpassword`*

   For security, your password is not displayed on the screen as you type it.

   If you make a mistake in typing your user name or password, the message
   `Login incorrect`
   appears and you are not given access to the system. In this case, you must reenter your user name and password.

   On systems using Solaris (unless CDE is running), if you attempt to log in and you do not yet have a password, the system informs you that you do not have a password and instructs you to choose one:
   `New password:`
   Follow the directions on the screen. The password must be at least six characters long and include at least two alphabetic characters and at least one numeric or special character (&, #, -, }, @, etc.).

   After your login is accepted, various system and user configuration files are read into memory to set up the system for you, including automatically starting VNMR software and displaying the VNMR interface.

   If you are configured as connected to a spectrometer and your system can perform acquisition, the Acquisition Status window and the Acquisition window should open without any further action on your part. Of course, if you are configured as a data station only (you are not connected to a spectrometer), these windows will not be useful to you.

3. If you want the Acquisition Status window to appear and it is not open, enter the command `acqstat` in the input window to start it.

   Alternatively, move the mouse arrow over the workspace (the background area not covered by any windows), then press and hold down the right mouse button until a pop-up menu appears. Continue to hold down the right mouse button while moving the mouse downward to highlight Acquisition Status, the first entry on the pop-up menu, then release the mouse button.

   Or, if CDE is installed, click on the button above the VNMR icon in the tool bar, then click on the Acqstat icon.

4. If you want the Acquisition window to appear and it is not open, enter the command `acqi` in the input window to start it.

   You must be connected to a spectrometer for this window to open.

To Exit VNMR

CAUTION: **Use only the following procedure to exit VNMR and log out. Any other method can cause lost or corrupted files.**

1. With the VNMR interface displayed, take one of the following actions:
   - If CDE is installed, click on the

button in the toolbar instead of following steps 1 through 5 to exit VNMR.
   - Enter in the input window the command `exit`.
   - Click on Main Menu | More | Exit VNMR

   If the Acquisition and Acquisition Status windows are present, both should automatically quit.
2. If the Acquisition Status window is still open, click on the EXIT button in the window to close the window and quit the program.

   You are now out of VNMR but still in the UNIX windowing system, logged in under your user name. In addition to the workspace (the background area not covered by any windows), you may yet have windows for some programs like a clock or a text editor still open and some icons on the screen for closed programs.
3. To close the windowing system, move the mouse arrow over the workspace and then press and hold down the right mouse button until a pop-up menu appears. Drag the mouse downwards until the Exit option at the bottom of the menu is highlighted and then release the mouse button.

   A dialog box appears with the prompt
   `Please confirm exit from window system`
   and two buttons: Exit and Cancel
4. Click on Exit with the left mouse button.

   The UNIX prompt for the current user appears, for example,
   `NMRlab:vnmr1>.`
5. Enter the command `logout`

   The login prompt appears, for example,
   `NMRlab console login:`

You are now logged out of the system.

2.2 Working with VNMR on the Host Computer

This section describes how the operator interacts with the system through a number of devices: the mouse, the keyboard, remote status module (not on all systems), and the display monitor. Each part of the VNMR screen is described in detail along with an introduction to working with Solaris and OpenWindows or CDE. Table 2 lists the commands and parameters discussed in this section.

Mouse Device

The mouse is a three-button pointing device that can be either mechanical or optical. The latest mouse design is a mechanical device with a rotating ball in its base. No special tracking board is required for this design; however, a mouse pad is useful.

When you move the mouse, a cursor correspondingly moves across the display screen. The cursor is most often a small arrow that tracks the movement of the mouse, that is, moving the mouse to the upper left moves the arrow to the upper left of the screen.

Table 2. VNMR Interface and Display Tools

Command	
`errlog`	Display recent VNMR error messages
`flip`	Alternately uncover and conceal `dg` program
`glide`	Display *GLIDE* interactive window
`large`	Use large graphics window
`small`	Use small graphics window
Parameter	
`errloglen` {integer}	Number of lines in VNMR error message display
`pslabel` {string}	Pulse sequence label shown in status window
Menu System	
GLIDE	Open *GLIDE* interactive window
Main Menu	Display the Main Menu
Flip	Alternately uncover and conceal `dg` program
Resize	Change size of graphics window

Mouse Buttons

The three buttons on the mouse, which are "clicked" by pressing down on them briefly, are used for different purposes by the software:

- The *left button* of the mouse (the button under the index finger of a right-handed person) is the generally the primary button. Selecting choices from menus, activating windows, positioning cursors, and similar actions are accomplished by clicking the left button or dragging the cursor with the left button held down.
- Within VNMR, the *center button* of the mouse is *always* associated with vertical scale—vertical scale of the spectrum, of the integral, of a 2D spectrum, etc.
- Within VNMR, the *right button* of the mouse is associated with the presence of a second cursor and is typically used for selecting expansions of 1D and 2D spectra.

The center and right mouse buttons are used with VNMR software only within the graphics window and when using the pulldown menus within the *GLIDE* user interface.

A special use of the left and right mouse buttons is in the Acquisition window such as setting the values of shims. If you move the cursor over a –#+ button (where # is a number, e.g., –1+) and then press the left button, the value shown reduces by the number on the button. If you press the right button, the value increases instead.

Specific functions will be described in conjunction with the relevant software. Note that these buttons serve other functions within the windowing environment provided by Sun, IBM, or SGI.

Keyboard

The operator enters commands, parameters, and other alphanumeric information into the data system through a keyboard. The keyboard is similar to keyboards used with other computers, with keys for letters and numbers, and a set of special keys, such as Control, Delete, Backspace, and Return. These special keys are particularly useful for editing commands in the input window. "Command Line Editing and Reentry" on page 96 covers this use of the keyboard.

There are also a series of function keys, labeled F1 through F9, on the top row of the keyboard. These functions keys can be used as an alternative to the mouse in selecting buttons in the VNMR menu system. This topic is discussed further below.

The two columns of keys on the left side of the keyboard (L1 to L10 on some keyboards) and the function keys F10 to F12 are not used in VNMR but can be helpful for working in the OpenWindows or UNIX environment. For example, positioning the cursor over a window and then pressing the Open (L7) key changes the window into an icon. To do the opposite, open an icon, position the cursor over the icon and press Open (L7). Or to move a window to the front of other windows, move the cursor over any part of the window and press the Front (L5) key.

Remote Status Module

The optional remote status module is a small enclosure with indicators and displays, usually placed next to the host computer display. Although considered here as part of the user interface, the remote status module actually connects directly to the NMR console, not to the host computer like the rest of the user interface.

The UNITY*INOVA* and UNITY*plus* versions of the module are shown in Figure 8. From top to bottom, the module contains the following indicators and displays:

- VT indicator displays the status of the variable temperature unit.
- Digital readout displays the temperature from the VT controller.
- Analog 0-to-100 meter displays the lock level.
- ACQ, LOCK, SPIN, PFG, and RCVR OVFL indicators display the status of acquisition, lock, spin, pulsed field gradient, and receiver overflow, respectively.
- XMTR, WFG, 0, 90, 180, and 270 indicators for CHANNEL 1 display the status of the transmitter, waveform generator, and phase information for channel 1. The same display appears for up to three more rf channels, depending on the number of channels configured on the system.

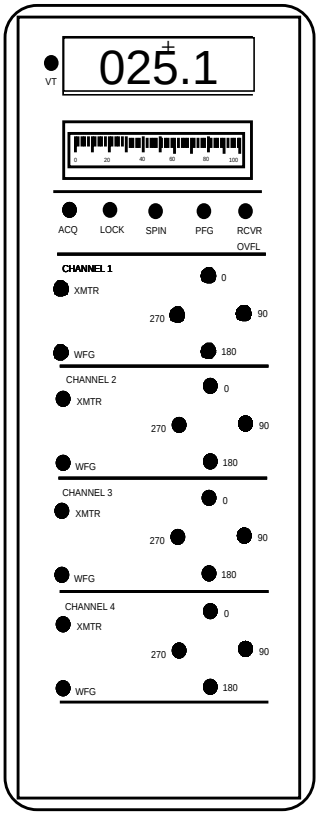


Figure 8. Remote Status Module

The UNITY version of the remote status module displays the status of lock, spin, observe transmitter, decouple transmitter, acquisition, and rf overload. In addition, the status for observe 90°, observe 180°, decouple 90°, and decouple 180° phase shifts are shown. The module also contains a lock level meter.

MERCURY-VX, *MERCURY*, and *GEMINI 2000* systems use a spin light and meter on the magnet leg. If the light is off, the sample is not spinning, If the light is flashing, the spin rate is not at the requested rate. If the light is steady, the spin rate is at the requested rate.

VNMR Display Screen

The VNMR display screen shows the operator what is happening with the data. Figure 9 shows a typical configuration of the windows in the display screen after logging in on a data station system (not configured for acquisition).

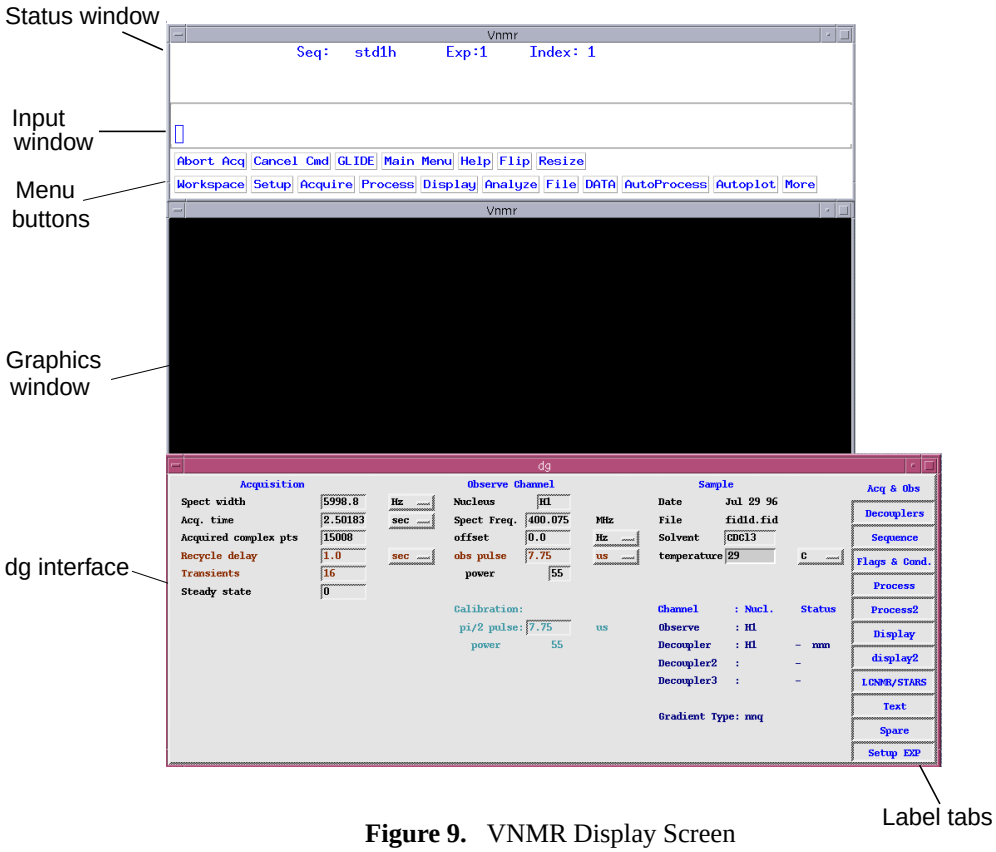


Figure 9. VNMR Display Screen

We will describe these windows according to their position in Figure 9, but like other windowing systems, you can move and close the windows as you want.

Standard Windows

The VNMR display screen contains a number of windows. At the top is the combined status, input, and menu system buttons windows. These windows appear as three separate windows when in use but can move as a single unit on the screen. In the middle of the screen is the graphics window. Below that is the dg program.

If the system is configured to perform acquisition, not just to be a stand-alone workstation, the right side of the screen often displays two other windows—the Acquisition Status window and the Acquisition window.

Status Window

On most systems, the status window occupies the top two lines of the VNMR display as well as a three-line scrollable window that appears below the top two lines. Figure 10 shows how a typical status window might look.

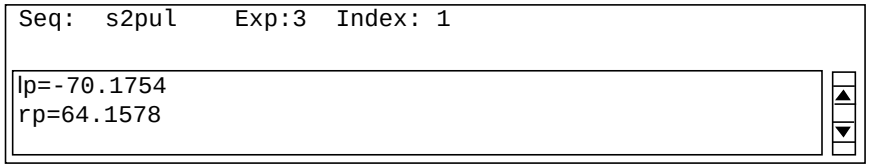


Figure 10. Status Window and Input Window

Each part of the status window displays important information about the system:

- The first line is a status line that informs the operator about the system action in progress. Near the center of this line is the name of the pulse sequence requested by the operator ("`Seq: s2pul`" in Figure 10). The sequence name is stored in the `pslabel` parameter. The status line continues with an indication of the current experiment number ("`Exp:3`" in Figure 10). This number refers to the experiment currently displayed on the screen, which is the experiment the operator can currently control. How the data system defines an experiment is discussed below. Short messages frequently appear on the right end of status line to identify the particular program that is executing, such as "`FT`" when a Fourier transform is in progress or "`CONT`" when a contour plot is being drawn.
- The second line displays the current plane during 3D data display. In the absence of 3D data, the second line is blank.
- The scrollable window is generally used to display system messages, such as "`Acquisition Complete`" or the value of a parameter, or to display error messages, such as "`Error in Input from Terminal`." The advantage of a scrollable window is that if a message has scrolled out of view, it can be retrieved by clicking on the scroll bar along the side of the window. You can edit text in this window by highlighting the text you want to copy or move using the left mouse button, and then pressing the right mouse button to pop up an Edit menu.

Only VnmrX installations feature the scrollable window. Other systems display a single line only. If VnmrX is installed on your system, you may want to change the size or even the existence of this window. To change the number of lines in the window, open the `/export/home/username/vnmrsys/app-defaults/vnmr` file or `/vnmr/app-defaults/Vnmr` with a text editor and change the number (preset at the factory to 1) at the end of the `*VNMR*errorLines` entry. To set the scrollable window to a single-line window, change the `*VNMR*errorLines` entry to 1 by preceding the line with the # character.

If the scroll bar is not there, the `errlog` command will display the last ten error messages in the `dg` program (the global parameter `errloglen` controls the number of lines displayed, ten lines is the default).

Note that the status window only provides information about the experiment in progress and does not reflect user input.

Input Window

Below the status window, enclosed in a box, is the input window. This window is the only place to type VNMR commands, and it must be active before you can type input.

On most systems, you activate the window by moving the mouse pointer into one of the VNMR windows and pressing the left mouse button. The cursor (a small box) becomes solid to indicate that the computer is ready for input from the keyboard.

As you type input, the cursor moves to the right indicating the current input position. Pressing the Return key terminates the end of one line of input. Commands can be strung together across the input block with spaces separating them. They can also be entered separately with Return pressed after each command. After Return is pressed, the computer checks the line you typed for correct syntax and then acts on the input.

Refer to Chapter 5, “Using the Command Mode,” , for a detailed description of entering commands and parameters into the input window, including editing your input from the keyboard.

Menu System Buttons

Below the input window are two rows of menu system buttons. Each row is considered a separate menu. Figure 11 shows a typical arrangement of the buttons on a data station (on a system configured as a spectrometer, an Acqi button appears): on the top is the Permanent menu, below that is the Main menu (which is displayed by clicking on the Main menu button in the Permanent menu).

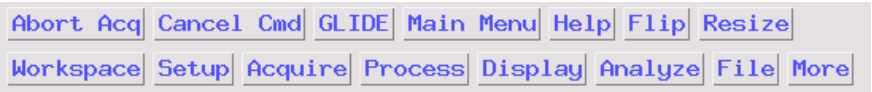


Figure 11. Menu System Buttons

To make a selection in the menu system, click on the desired menu button with the left button of the mouse. The menu system is organized so that the menu and button you most likely will need is on view, but if the button you want is not visible, clicking a series of buttons should bring it into view.

For example, one way to exit VNMR is to click on the Exit VNMR button, but if the menus displayed on your screen appear the same as shown in Figure 11, the Exit VNMR button is not on view. You quickly realize that clicking on the More button in the Main menu makes a new menu appear that includes Exit VNMR as the fourth button (labeled as Exit VNMR). This means that to exit VNMR you should click on Main menu, then click on More, and finally click on Exit VNMR.

As a shorthand notation to describe this action in VNMR manuals, we will write **Main Menu** > **More** > **Exit VNMR**. Chapter 4, “Using the VNMR Menu System,” describes all of the buttons in the standard menus.

The label and action for all buttons in the VNMR menu system can be customized for local use. The procedure is described in the manual *VNMR User Programming*.

Graphics Window

Below the menu buttons is the main VNMR graphics window. In this window are displayed FIDs, spectra, contour plots, and other types of NMR data. The graphics window also displays files when the File button in the Main menu is selected. Specific commands that display information in this window are explained throughout this manual, with instructions as to how to interact with the displayed information.

The graphics window can be either small, in which the graphics window and the `dg` program can be viewed at the same time, or large, in which the graphics window covers the full screen. You can change sizes through the menu system or by entering a command in the input window:

- To enlarge the graphics window to fill the screen, select the Resize button in the Permanent menu or enter the `large` command.
- To reduce the size of the graphics window to the small size, select the Resize button in the Permanent menu or enter the `small` command.
- To alternately uncover and conceal the `dg` program when it is covered by the graphics window, click on the Flip button in the Permanent menu or enter the `flip` command.

If VNMR is busy executing a command, the mouse pointer becomes a miniature clock or hourglass when positioned over the graphics window.

dg Program

At the bottom of the screen is the `dg` program, which is used to display parameter lists, line lists, help files, and other alphanumeric information. For example, entering the `dg` command in the input window produces a display of acquisition and processing parameters and their values in the `dg` program similar to Figure 12.

```
   ACQUISITION            SAMPLE            PROCESSING            FLAGS
sfrq       500.618  date     March 8, ~ lb          50.00  il              n
tn              H1                1995  sb        not used  in              n
at           2.305  solvent      cdcl3  gf        not used  dp              y
np           29952  file           exp  awc       not used  hs             nn
sw          6497.7      DECOUPLING      lsfid     not used       SPECIAL
fb            3600  dn               H1  phfid     not used  temp      not used
bs        not used  dof            74.7  wtfile
ss               0  dm              nnn  proc            ft
pw            23.0  dmm               c  fn        not used
p1               0  dmf             200  math             f
d1               0  dlp              20
d2               0                      werr         react
tof         1100.0                      wexp      procplot
nt              16                      wbs
ct               0                      wnt            wft
```

Figure 12. Typical Parameter Display in `dg` Program

Tcl Version of dg Window

The Tcl (Tool Command Language) version of the `dg` program resides in the `tcl/bin` directory of the VNMR system directory. A Tcl script can be sent to the Tcl version of the `dg` window that makes the entries in the display interactive and allows customization of the layout.

The `dg` program is strictly an *output* window; text input occurs only in the input panel near the top of the screen. Some output to the `dg` program might produce more information than can be displayed on a single screen. In this case, a scroll bar appears along the edge of the window. (On some systems, the scroll bar is always present.) Click on the scroll bar with the mouse to retrieve material that has scrolled out of view.

You can edit text in this window by highlighting the text you want to copy or move using the left mouse button, and then pressing the right mouse button to pop up an Edit menu.

If the Tcl version of the `dg` window is not active, the `tcl` command does nothing For more information about Tcl scripts, see *VNMR User Programming*.

Selecting the Interactive dg Window

The `dg` interface is selected by setting the UNIX environmental variable `vnmrtext` to the full path of the `dg` program. The following line in the `.login` file selects the interactive `dg` window:

```
setenv vnmrtext $vnmrsystem/tcl/bin/dg
```

Deselecting the Interactive dg Window

If you comment out the previous line with a # character in front of it, the noninteractive `dg` window will be selected.

Configuring the dg Window

The `dg` window has a built-in configuration tool. You can activate this tool by simultaneously holding down the **Control** key and pressing the left mouse button over a label tab. Use this tool to move items around on the dg window and create or remove new items. For more information about configuring the `dg` window, see "Customizing the Interactive dg Window" in chapter 6 of the *User Programming* manual.

CONSOLE and VNMR Shell Windows

If OpenWindows is running, in the upper right-hand corner of a typical VNMR screen display are two icons for shell windows, CONSOLE and VNMR, as shown in Figure 13. Under CDE, these icons are not needed.

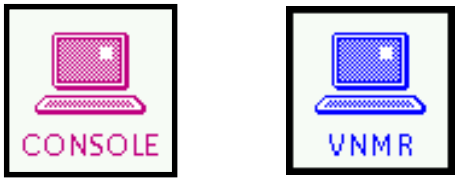


Figure 13. CONSOLE and VNMR Shell Windows

The CONSOLE shell window is automatically created when OpenWindows is started at login time (do not confuse this window with the NMR console). This window is used by the UNIX operating system to display diagnostic messages such as "`su command succeeded for user A`" or "`starting Acqproc`." To see these messages, double click the CONSOLE icon with the left mouse button. Do not quit the CONSOLE shell window; otherwise, system messages are written to the background or workspace, causing the window graphics to scroll off the screen. However, if you are using CDE, you can quit this window.

The VNMR shell window icon is also automatically created when OpenWindows is started. Because every UNIX command must be started from a shell window, the Vnmr command to start VNMR is entered in this window. Certain diagnostic messages from Vnmr are displayed in the VNMR window. Again, do not quit this window. However, if you are using CDE, you can quit this window.

For details about these windows under OpenWindows, see the file `.openwin-init`.

Optional Windows

In addition to the standard VNMR windows described above, many other windows are possible, some of which you will use so frequently that you may want to make them appear automatically when you enter VNMR. Perhaps the most important optional windows from VNMR are the Acquisition window and the *GLIDE* user interface. Many other options are available from the Workspace menu that pops up from the workspace, including VNMR Online, Shell Tools, Clock, and Performance Meter.

Acquisition Windows

If the system is not just a stand-alone workstation but is connected to a spectrometer, the right side of the screen can be used for two optional acquisition windows:

- The Acquisition Status window displays information about the status of data acquisition: Is data being acquired or is the system idle? How many transients have been completed (CT), and what is the estimated completion time of the experiment? What is the spinning speed? What is the lock level? The Acquisition Status window is strictly an output window. Use of this window is described in Chapter 4.
- In the Acquisition window, you have the ability to interact with the acquisition console. On UNITY*INOVA* systems, this window can be present at any time. On other systems, it can only be active ("`CONNECTED`") when an acquisition is not in progress. In the Acquisition window, the mouse can be used to eject and insert samples (if the hardware is available), turn the spinner on and off, adjust the lock channel, and adjust the various shim gradients. Use of this window is described in Chapter 3.

Both acquisition windows open automatically when you enter VNMR if your system is configured for acquisition (not a data station). To otherwise open and close these windows, see "Entering and Exiting VNMR" on page 39.

GLIDE Interactive Acquisition and Processing Window

The *GLIDE* interactive data acquisition and processing window, shown in Table 14, is activated by clicking on the GLIDE button in the Permanent menu or by entering the `glide` command in the input window.

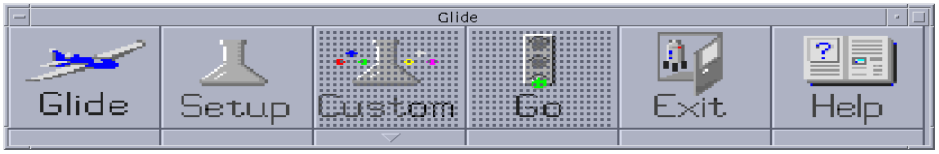


Figure 14. *GLIDE* User Interface Window

Refer to Chapter 3, "Using GLIDE," for a detailed description of the *GLIDE* window.

Workspace Menu

Many windows for programs are accessible from the pop-up Workspace menu, shown in Figure 15.

To open the Workspace menu and make a selection:

1. Move the mouse arrow over any part of the workspace area of the screen (where no windows appear).
2. Press and hold down the right mouse button until the Workspace menu appears.
3. Continue to hold down the right mouse button and drag the cursor to the item you want.
4. If the item you want has *no* small triangle to the right of it, simply release the mouse button to select that item. After several seconds, the window appears for the program you wanted.

Figure 15. Workspace Menu under OpenWindows

If the item you want has a small triangle to the right of it (that is, the Programs and Utilities items on the Workspace menu), that item has a submenu. To open the submenu, continue to hold down the right button and slide the mouse toward the right of the item, across the triangle, until the submenu opens, then move the cursor to the item you want on the submenu and release the button.

Here are some programs accessible from the Workspace menu that you will probably frequently use:

Acquisition Status	Opens the Acquisition Status window, one of the VNMR acquisition programs discussed above.
VNMR Online	Displays hypertext version of all your VNMR user manuals including all the entries in the *VNMR Command and Parameter Reference* and all the pulse sequence statements in the *VNMR User Programming* manual. Many users leave this program on all the time for quick retrieval of useful operating information.
Vnmr	Activates the VNMR display window. If the VNMR display is already active, selecting Vnmr creates a second instance of the display (probably useless, click on ExitVNMR to quit).
Programs	Opens a submenu with more choices, including these useful programs:
Shell Tool	Allows you to interact with the UNIX operating system. Many users find a Shell Tool window the fastest way to copy, delete, create, and edit files, do backups, write macros, change passwords, monitor processes going on at the host computer, and so on.
Clock	Displays a clock that can be set many different ways, for example, as either analog or digital. Click on the clockface with the right mouse button to open the Clock Properties menu that allows customization.
Performance Meter	Gives you an indication of how hard the CPU of your computer is working and is useful as a monitor of what processes are going on in the background.

CDE Menu

Programs can also be accessed from the CDE toolbar, shown in Figure 16.

Figure 16. CDE Toolbar

Closing and Opening Windows

Each of the windows on the screen can be closed and changed to a small icon. When closed, each window changes to a small, distinctive icon, as shown in Figure 17. This can be useful when many windows are open and you would like more screen space.

To close a window on Vnmr, move the mouse cursor to the line on the edge of the window and click the right mouse button until a popup menu appears. Select Close from the menu. Alternatively, you can move the cursor within the window you want to close and then press the Open key (L7 on some keyboards) on the keyboard.

Figure 17. Icons for Closed VNMR Windows

To open any of these icons, move the mouse arrow over the desired icon and either double click the left mouse key or press the Open key (L7) on the keyboard.

CAUTION: ***You could exit the VNMR application from the closed icons, but do not exit this way.*** **The VNMR program keeps data and parameters in internal buffers. If you exit from a closed icon, the buffers will not be written to the hard disk and data will be corrupted or lost.**

The correct way to exit from VNMR is to reopen the combined status and input window (the icon containing the word “Master” four times) and then follow the procedure in “Entering and Exiting VNMR” on page 39.

Chapter 3. Using *GLIDE*

Sections in this chapter:

- 3.1 “Activating GLIDE” this page
- 3.2 “Using GLIDE” page 54
- 3.3 “Customizing Combination Experiments” page 56

GLIDE is a user interface designed for walk-up NMR use. It facilitates setup, acquisition, processing, and plotting tasks.To customize *GLIDE*, refer to the manual *Walkup NMR Using GLIDE*, which contains a more detailed description of this interface.

3.1 Activating *GLIDE*

When you open the *GLIDE* interface, shown in Figure 18, the menu overlays the top of the VNMR window.

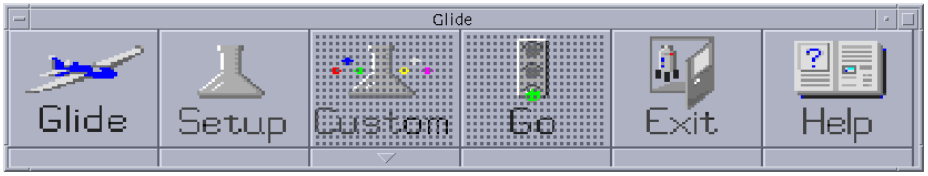


Figure 18. *GLIDE* User Interface Window

After *GLIDE* has been activated, the *GLIDE* button in the Permanent menu acts as a toggle, allowing the *GLIDE* window to be moved into view or hidden behind other windows.

Opening *GLIDE*

To open the *GLIDE* user interface window, do *one* of the following actions:

- Click on the ***GLIDE*** button on the Main Menu.
- Enter the command **`glide`** in the VNMR input window.

Closing *GLIDE*

To remove the *GLIDE* user interface window from the display but keep the program running, click on the ***GLIDE*** button in the VNMR Permanent menu. To bring back the *GLIDE* window, click again on the ***GLIDE*** button or enter the command **`glide`**.

To close the *GLIDE* program so it no longer is running, take one of the following actions:

- Click on the **Exit** button.
- Enter the command **`glide('exit')`**.

You might be asked to confirm that you want to exit *GLIDE*. Customizing the file `glide_defaults` (described in the manual *Walkup NMR Using GLIDE*) determines whether or not you see the confirmation window.

3.2 Using *GLIDE*

The *GLIDE* interface makes obtaining spectra on the system extremely easy. Each experiment accessed from the Setup button can be run in exactly the same manner. Only three simple steps are required to run each experiment on the list:

- Insert your sample.
- Choose the experiment and solvent via the Experiment Setup window.
- Click on the Go button.

GLIDE contains a nonfunctional icon box (labeled *GLIDE*) and six buttons: Setup, Custom, Go, Exit, and Help. For descriptions of each of these buttons, refer to the *Walkup NMR Using GLIDE* manual.

Running a Standard Experiment

A typical session with *GLIDE* is described in the following step-by-step procedure for running a 1D proton NMR in deuterochloroform.

1. If the *GLIDE* user interface is not displayed, click the ***GLIDE*** button in the Permanent menu.
2. In the *GLIDE* user interface, click on **Setup**.

   The Experiment Setup window appears on the screen.
3. Using the right mouse button, click on the menu button labeled **Experiment**.

   A menu with a list of available experiments is displayed.
4. Scroll through the experiment list by holding down the right mouse button and dragging the pointer through the choices. Release the right mouse button when the **Proton 1D** option is highlighted.
5. Using the right mouse button, click on the menu button labeled **`Solvent`**.

   A menu with a list of available solvents pops up.
6. Scroll through the solvent list by holding down the right mouse button and moving the pointer through the choices. Release the right mouse button when the **CDCl3** option is highlighted.
7. If you want to enter a file name for saving the data or enter text for your sample, click on the field labeled **Save As** with the left mouse button and begin typing.

   To enter text, which will be printed along with parameters on the spectrum, click in the box below the label Text. One click positions the insertion point (and cursor) at that spot in the text. Two clicks highlights the single word under the pointer. Three clicks highlights the entire line. Four clicks highlights the entire text. In all cases, highlighted text is deleted and replaced as soon as you type any character (including the space bar). Multiple line texts are supported.
8. If your system has automatic insert and eject capability, buttons for insert and eject appear in the window:

- If a sample is currently in the magnet, click on the **Eject** button to eject the sample. Next, insert your sample and click the **Insert** button to insert the sample into the magnet.
- Alternately, if a sample changer is attached to your system, enter the location of the sample in the sample tray, using the field labeled **Location**.
- If you do not have the auto insert and eject feature on your spectrometer, the Insert and Eject buttons are not displayed and you need to manually insert your sample.

9. Click the **Setup** button to exit from the Experiment Setup window.

   Acquisition does not begin at this point. *GLIDE* is only setting up parameters. Once you click Setup, the Experiment Setup window disappears, the Custom and Go buttons become active, and the Custom Setup window appears.

10. To use default values, click on **Go** in the *GLIDE* interface to acquire a spectrum.

    The system will autolock, autoshim, acquire, process, and plot the data using the default parameters.

enter Program

GLIDE experiments can also be accessed from the `enter` program. The experiment file created by `enter` is now saved in a directory of the same name. For example, the command `enter('abc')` creates a directory named `abc`. A file named `abc` and another directory named `abc.macdir` will be in that directory. `abc` has the experiment information, and `abc.macdir` has *GLIDE*-related information for the automation run.

Customizing a 1D Experiment

In addition to the previously outlined scenario, *GLIDE* permits you to customize experiments to obtain, for example, a spectrum with a greater number of scans than the default. As an example, assume that the default number of scans for carbon 1D on the system is 1024. Your sample, however is quite concentrated and you need only 16 scans. You can set up the carbon 1D experiment and modify the number of scans using *GLIDE*:

1. Follow steps 1 through 9 in the “Running a Standard Experiment” on page 54, but instead of choosing Proton 1D, choose **Carbon 1D** in step 4.

   The Custom Setup window appears. This window has four buttons that each open an associated setup window with parameters that can be changed. These windows permit the user to perform in two different modes of operation:

   In the first mode, you customize acquisition, processing, and plotting parameters displayed in the setup windows prior to initiating acquisition with the Go button. By clicking the Close button in each setup window, the setup window is closed and the parameter values are saved. We will use this mode in the following steps.

   In the second mode, you also change parameters, but by clicking on the Do button in *each* setup window, you immediately acquire (or reacquire) data, process the data with specified parameters or plot the data with the specified parameters. (Note that each setup window is separate and immediate: clicking on Do in the Acquire Setup window only acquires, clicking on Do the Process Setup window only processes, and clicking on Do in the Plot Setup window only plots. This allows you to easily explore the effect of changing parameters.)

2. Click on the **Acquire Setup** button in the Custom Setup window. The Acquire Setup window is displayed with the Number of Scans set to 1024.0 (if this item is not on

view, use the scroll bar on the right side of the window to scroll it into view). In this example, change the number of scans from 1024 to 16 by clicking on the line at the end of the number and using the Back Space key to delete the current value. Type in the new value of 16.

3. When you are done, click on the **Close** button to exit and save the change. *Do not click on the Do button at this point unless you wish to acquire data immediately.*

   Clicking on Do after making a change is the equivalent of entering the `go` command in which acquisition begins but no further processing is performed.

4. Click on the **Process** button in the Custom Setup window. The Process Setup window appears with the current values of the Fourier Number and Line Broadening. To change the value displayed, delete the number with the Back Space key, type a new value, and click the Set button.

5. When you are done, click on the **Close** button to save any changes and exit. *Do not click on the Do button unless you wish to process the data immediately with the parameters you have chosen* (this feature lets you easily reprocess data already in the experiment).

6. Click on the **Plot** button in the Custom Setup window. The Plot Setup window appears for customizing plot layouts. Make the changes you want.

7. When you are done, click on the **Close** button to save any changes and exit. *Do not click on the Do button unless you wish to plot the data immediately with the parameters you have chosen* (this feature lets you easily make additional plots of your processed data).

8. Exit the Custom Setup window by clicking on the upward-pointing triangle at the bottom of the Custom button in the *GLIDE* user interface window.

9. Now that you have chosen all the parameters for acquisition, processing, and plotting, click the **Go** button in the *GLIDE* user interface to initiate acquisition.

   The data will be acquired, processed, and plotted using the values set within the Custom Setup windows.

3.3 Customizing Combination Experiments

In addition to setting specific parameter values in 1D experiments, *GLIDE* allows you to select an arbitrary combination of values from a list of available experiments and separately customize each selected experiment. As an example, to run 1D proton, COSY, and HMQC experiments on a sample, do the following steps:

1. Open the Experiment Setup window, as described in “Running a Standard Experiment” on page 54.

2. Select **H1 and H1 detected Experiments** from the Experiment menu.

3. Enter a name in the **Save As** field. Your entry will be appended to the directory name in which all data will be stored, i.e., `~vnmrsys/data`.

4. Click on **Setup** to retrieve standard proton parameters and activate the Custom menu.

5. Click on the **Acquire** icon to open the Acquisition Setup window.

6. Select the spectral window, number of transients, relaxation delay and pulse angle for your sample. The spectral window you choose will be used for all experiments; the other selections are used only for the 1D spectrum.
7. Click on the **COSY** button in the top row of the experiment selection menu.
8. In the new window, shown in Figure 19, use the left mouse button to choose the number of transients per increment and the number of increments in the COSY experiment. The values that you choose are shown as depressed buttons.

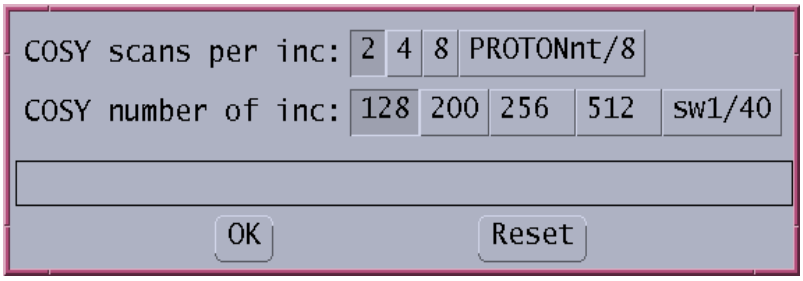


Figure 19. COSY Customization Window

9. When you have made your choices, click the **OK** button in the popup window to close it and add the COSY experiment to the experiment list. The list is displayed in the VNMR text window and now has the entries PROTON and COSY.
10. Click on the **HMQC** button in the middle row of the experiment selection menu to open the HMQC customization window shown in Figure 20.

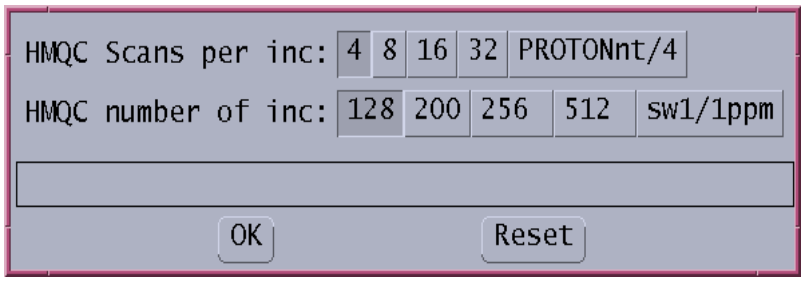


Figure 20. HMQC Customization Window

11. Make your selections and click on **OK** to add the HMQC experiment to the list that appears in the VNMR text window.
12. Click on the **Close** button to remove the Acquisition Setup window.
13. Click the upward-pointing triangle, at the bottom of the Custom icon, to close the Custom menu.
14. Click the **Go** button in the main *GLIDE* menu.

Processing and Plotting Combination Experiments

Some processing and plotting automatically happens in *GLIDE* combination experiments. The 1D proton spectrum is always processed and plotted, as is a COSY (if it is run). Phase-sensitive experiments are saved in the data directory for this sample (specified in the Save As field in the setup window). To process and plot these experiments, the data must be

recalled and specific plotting actions must be taken. Data can be recalled and processed with either Common Desktop Environment (CDE) or VNMR menus.

Recalling Data in CDE

Before recalling data, the VNMR command `listenon` must have previously been given (once is sufficient) for the procedure to work.

To recall data with the CDE FileManager, do the following steps:

1. Change to the directory in which the data was stored.
2. Double-click the icon for the desired data (FID) to load and process the data, using processing parameters (including the name of the processing macro) which were stored with the data set. *The OpenWindows FileManager cannot be used for this purpose.*

Recalling Data Using VNMR Menus

To recall and process data using VNMR menus, do the following steps:

1. Click on the **Main Menu** button in the Permanent menu.
2. If you are not already in the data directory, click on the **DATA** button in the second-level menu. If you are already in the desired directory, choose **Files** from the second-level menu.
3. If you used the DATA button, find the name of the directory containing the data you want to recall and highlight it by clicking on it with the left mouse button.
4. Click on **Set Directory** in the second-level menu.
5. Find the name of the data file you wish to load, highlight it, and click the **Load** button in the second-level menu to recall data and processing parameters, including any processing macro names.
6. To process the data, click on the **Main Menu** button in the top-level menu and then click on the **AutoProcess** button in the second-level menu.

   After the data has been processed, you are left in the appropriate interactive display (1D or 2D), where you can adjust the expansion, vertical scale, or threshold before making the plot. Refer to the *User Guide: Liquids* for details of the interactive 2D display.
7. When the display has been adjusted to your satisfaction, click on **Autoplot** in the second-level menu to plot the currently displayed portion of the spectrum.

   If high-resolution 1D spectra are available (in the current data directory), they will be plotted along the edges of the 2D spectrum to aid in interpretation.

Walkup NMR

Refer to the *Walkup NMR Using GLIDE* manual for detailed instructions on how to perform “walkup NMR” experiments and system calibrations using the *GLIDE* interface.

Chapter 4. Using the VNMR Menu System

Sections in this chapter:

- 4.1 “Working With Menus” page 60
- 4.2 “Customizing the Menu System” page 64
- 4.3 “Menu System Step-by-Step” page 64
- 4.4 “Permanent Menu” page 65
- 4.5 “Main Menu” page 66
- 4.6 “Workspace Menu” page 67
- 4.7 “Setup Menus” page 67
- 4.8 “Acquire Menu” page 70
- 4.10 “Display Menus” page 77
- 4.11 “Analyze Menus” page 81
- 4.12 “File Menus” page 87
- 4.13 “Secondary Main Menu” page 91

Like most software, the VNMR software package can be operated by using a keyboard to type in commands and parameters, thus causing spectra to be acquired, processed, plotted, etc. But VNMR software also includes an extensive series of menus, which at any time provide a number of buttons that allow access to the essential functions of operating an NMR spectrometer—experiment setup, acquisition, data processing, display, plotting, analysis, and more. Many users will be able to operate their spectrometer for hours at a time with little or no resort to the keyboard.

The VNMR menu system provides an excellent mechanism for new users to begin acquiring or processing data with little or no training. It isn’t necessary to know that `wft` is the command that performs a weighting of the FID and a Fourier transform, because the button marked Weight,Transform is self-explanatory. It also isn’t necessary to know that `dpcon` to displays a 2D contour plot, because a button marked Contour Plot is available.

Using the buttons is simplicity itself—move the mouse arrow or cursor to a point over the desired menu button, then click (press the mouse button and release) the left button on the mouse. The function keys F1, F2, or F8 etc. on the keyboard can be used as an alternative method for selecting the first eight menu buttons on all menus except the Permanent menu (described in the section “Permanent Menu” on page 65): key F1 selects menu button 1, F2 selects button 2, F8 selects button 8.

Despite the user-friendly labels on the menu buttons, you may be unclear about what a particular button choice will do. Clicking on the button labeled Help in the Permanent menu (which is always available) causes a help screen to be displayed in the text window. This screen provides an explanation of each of the menu buttons and explains the function of the three buttons on the mouse for the menu buttons on view.

4.1 Working With Menus

At all times, two rows of menu choices are accessible to you on the screen. The upper row, which can be selected only by using the mouse (and not by function keys), is the Permanent menu. Although the labels and actions of these buttons are customizable (see the manual *VNMR User Programming*), their functions do not change during a VNMR session.

Located below the Permanent menu is another row of up to 20 buttons whose choices vary depending upon which menu is on display. The default is the Main menu, which contains the following buttons:

The Main menu can always be activated by clicking on the Main menu button in the Permanent menu. You can make selections in the Main menu by either clicking on the button or by pressing one of the F1–F8 keys, for example, to select Setup, press F2.

Making a selection on the Main menu causes a different set of buttons to replace the Main menu. For example, if you select the More button, the following extension of the Main menu, called the Secondary Main menu, replaces the Main menu:

By clicking on the Return button (or pressing F5) in the Secondary Main menu, the Main menu now replaces the Secondary Main menu—you are back where you started.

Similarly, you can display dozens of menus, each with buttons capable of certain actions affecting system operation. For reference, Table 3 outlines the *default* version of the VNMR menu system (see "Customizing the menu System" below). Menu buttons that call another menu are underlined in the list.

If your prefer, you can also call up a particular menu by typing `menu(menu_name)`, where `menu_name` is the name of the menu (e.g., `menu('workspace')` calls up the Workspace menu). Some menus have a separate command; for example, entering the command `files` displays the Files Main menu. For the names of menu files, look in the `/vnmr/menulib` directory.

Note that selecting a particular button may produce more than one action, depending on the current value of certain parameters, the nature of the data, or any other identifiable factor. For example, in the case of the Main menu, the Process and Display buttons both first look to see whether the experiment holds 1D or 2D data, and then display a 1D or 2D menu appropriate to the experiment.

Interactive Programs with Menus

The VNMR software contains a number of interactive programs—`dconi`, `df`, `ds`, `ll2d`, etc.—with menus that operate the same as the main menu system. Table 3 includes these programs and menus. To run these programs, enter the program name (e.g., `dconi`). Since these programs are integrated into the main menus system, each can also be called from one or more of the buttons in the menus listed in Table 3.

Table 3. VNMR Menu System (Part 1 of 4)

Note: Underlined button labels means that the button displays another menu.

Permanent Menu (always present), page 65
Abort Acq, Cancel Cmd, GLIDE, Main Menu, Help, Flip, Resize Acqi

Main Menu (from Main Menu button in Permanent menu), page 66
Workspace Setup Acquire Process Display Analyze File More

Workspace Menu (from Workspace button in Main menu), page 67
Library Exp2 Exp3 Exp4 Exp5 Exp6 Create New Delete

Setup Menu (from Setup button in Main menu), page 67
H1,CDCl3 C13,CDCl3 Nucleus,Solvent Sequence App Mode Acquire

Nucleus Selection Menu, page 68
H1 H2 C13 N15 F19 P31 Other Return

Solvent Selection Menu, page 68
CDCl3 D2O Benzene DMSO Acetone Other Return

1D Pulse Sequence Setup Menu, page 68
APT DEPT INEPT BINOM S2PUL More ID 2D Return

1D Pulse Sequence Setup Secondary Menu, page 69
D2PUL SSECHO XPOLAR More 1D 2D Return

2D Pulse Sequence Setup Menu, page 69
COSY COSYPS HETCOR NOESY ROESY 1D More 2D Return

2D Pulse Sequence Setup Secondary Menu, page 70
DQCOSY HET2DJ INADQT HOM2DJ TOCSY 1D More 2D Return

Applications Mode Menu, page 70
Standard Imaging Return

Acquire Menu (from Acquire button in Main menu), page 70
Show Time Go Go,Wft Go,Periodic Wft Automatic

1D Data Processing Menu (from Process button in Main menu), page 71
Display FID Select Params Adj Weighting Transform Weight,Transform

Interactive 1D FID Display Menu—df program, page 71
Box Imaginary Expand sf wf Dscale Phase Return

1D Processing Parameter Setup Menu, page 72
No WT Resolve Broaden ->AV FN:Small Normal Large Return

Interactive Weighting Menu—wti program, page 72
next fid lb sb sbs gf gfs awc return

Interactive 1D Spectrum Display Menu—ds program, page 73
Box Part Integral Full sp wp Mark Phase Next Return

(***continued on next page***)

Table 3. VNMR Menu System (Part 2 of 4)

2D Data Processing Menu (from Process button in Main Menu), page 73
Select Params Adj Weighting Phase F2 Transform F2 Full Transform

2D Processing Parameter Setup Menu, page 73
No WT Sinebell Pseudo ->PH FN:Small Normal Large Return

2D Interferogram Processing Menu, page 74
Color Map Adj Weighting F1 Transform Reprocess

Interactive Weighting Menu—wti program, page 72
next fid lb sb sbs gf gfs awc return

Interactive 2D Color Map Display Main Menu—dconi program, page 74
Box Trace Proj Expand Redraw Plot Peak Return

Interactive 2D Display Projection Menu—dconi program, page 75
Hproj(max) Hproj(sum) Vproj(max) Vproj(sum) Plot Cancel

Interactive 2D Peak Picking Main Menu—ll2d program, page 75
Auto Edit File Display Return

2D Peak Picking Automatic Menu—ll2d program, page 75
Box Peak Volume Full Both Adjust Reset Return

2D Peak Picking Edit Menu—ll2d program, page 76
Box Mark Unmark Full Clear Combine Next Return

2D Peak Picking File Menu—ll2d program, page 76
Read Read Text Write Text Backup File Return

2D Peak Picking Display Menu—ll2d program, page 76
Hd Pk Hd Num Hd Box Hd Lbl Sh All Hd all Return

1D Data Display Menu (from Display button in Main menu), page 77
View Interactive Massage Size Reprocess Plot More

1D Data Manipulation Menu, page 77
DC Region BC Autophase Adj VS Adj IS Adj WP Return

1D Display Size Selection Menu, page 78
Left Center Right Full Screen Return

1D Plotting Menu, page 78
Plot Scale HP Params Params All Params Peaks Page Return

1D Data Display Secondary Menu, page 78
Lines Integrals Dssh Dssa AV Reference Return

2D Data Display Menu (from Display button in Main menu), page 79
Color Map Contour Image Size Massage Reprocess Plot More

2D Display Size Selection Menu, page 79
Left Center Right Full Screen Full with Traces Return

2D Data Manipulation Menu, page 79
DC(f2) DC(f1) Foldt Foldj Foldcc Rotate Normalize Return

2D Plotting Menu, page 80
All Contours Pos. Only Image All Params Params Page Return

2D Data Display Secondary Menu, page 80
Stacked Plot F2 Mode PH Reference Analyze Return

(*continued on next page*)

Table 3. VNMR Menu System (Part 3 of 4)

Analyze Menu (from Analyze button in Main menu), page 81
Exponential DEPT COSY Add/Sub Simulation Deconvolution Regrs

Exponential Analysis Menu, page 81
T1 Proc T1 Analysis T2 Proc T2 Analysis Plot Print Return

Automatic DEPT Analysis Menu, page 81
Process Display Plot Edit Printout Full Analysis Return

Automatic COSY Analysis Menu, page 82
2D Line List Find Correlations Plot Correlations Redisplay Return

Add/Subtract Menu, page 82
Clear Interactive Mode Add Spectrum Subtract Minimum

Interactive Add/Subtract Menu—addi program, page 83
Box Select Expand sp wp sub save return

Spin Simulation Main Menu, page 83
Spin System Show Params Set Params Simulate Original Next

Spin Simulation First Definition Menu, page 83
AB ABC A2B ABCD A2BC A3B other return

Spin Simulation Second Definition Menu, page 84
ABCDE A2BCD A3BC A2B2C A3B2 A3B2C other return

Spin Simulation Third Definition Menu, page 84
AX AXY AX2 AXYZ AX2Y AX3 other return

Spin Simulation Secondary Menu, page 84
list params assign display iterate observe :return main

Spin Simulation Line Assignment Menu, page 85
ll use ll use fitspec auto assign iterate return main

Deconvolution Menu, page 85
Use Line List Use Mark Fit Results Show Fit Plot Add/Sub

Regression 1 Menu, page 86
x-linear x-square x-log dp-linear dp-quad dp-exp next Rt

Regression 2 Menu, page 86
y-linear y-square y-log dp-linear dp-quad dp-exp Next Rt

Regression 3 Menu, page 86
dp-linear dp-quad dp-cubic dp-exp plot dp output Return

Files Main Menu (from File button in Main menu), page 87
Set Directory File Info Tape Load Data Delete More Return

Directory Menu, page 88
Change Default Set Default Parent Home Nmr More Return

Directory Secondary Menu, page 88
NMR Create New Return

Files Information Menu, page 89
By Size By Date Return

Files Tape Menu, page 89
Directory Sizes Write Read All Return

Files Data Menu, page 90
Load Save FID Show Shims Load Shims SaveShims More Return

Files Data Secondary Menu, page 90
Load Params Save Params Return

Files Secondary Menu, page 90
Display Edit Copy Rename Return

(***continued on next page***)

Table 3. VNMR Menu System (Part 4 of 4)

Secondary Main Menu (from More button in Main menu), page 91
Write Pulse Sequence Configure UNIX Exit VNMR Return

Pulse Sequence Entry Main Menu (see *VNMR User Programming*)
Start Delay Pulse DecPulse Status Other Finish Show Seq.

Pulse Sequence Entry Delay Menu (see *VNMR User Programming*)
D1 D2 D2/2 D3 MIX Allow Homospoil Return

Pulse Sequence Entry Phases Menu (see *VNMR User Programming*)
SELECT PHASE: Use Previous X Y –X –Y Fixed:0 +-+- More

Pulse Sequence Entry Phases Secondary Menu (*VNMR User Programming*)
3210 0321 0022 2200 Fixed:90 Fixed:180 Return

Pulse Sequence Entry Pulses Menu (see *VNMR User Programming*)
PW P1 2PW 2PI Other Return

Pulse Sequence Entry Decoupler Pulses Menu (see *VNMR User Programming*)
PP 2PP Other Return

Pulse Sequence Entry Status Menu (see *VNMR User Programming*)
A B C D RcvrOn RcvrOff Set Rcvr Phase Return

Configuration Menu page 92
Show Output Devices Select Plotter Select Printer Hardware Return

4.2 Customizing the Menu System

Most of the menus and help files for the menu system can be customized for local use. Information on how to customize the menus and help files is provided in the manual *VNMR User Programming*. The description of menus and help files in this manual applies to the default version supplied with the software.

4.3 Menu System Step-by-Step

The following example takes you through the process of recalling some stored data, processing it, displaying it, and plotting it. Go through it once exactly as described to get a feel for operating the system. Then go through it again, trying some of the different choices that were available to you along the way. You might also try going through the example using the function keys instead of the mouse.

1. In the Permanent menu, click on **Main menu**.
2. Starting from the Main menu (the lower row of buttons), click on the following buttons: **File** > **Set Directory** > **Parent**.

   The graphics window shows a list of directories (entries with a slash as last character) and files (if any). The status window (at the top of the screen) shows the pathname of the directory you are in currently.
3. Click as many times as necessary on the **Parent** button until the message "`Directory now /`" appears in the status window.
4. Click the mouse on `vnmr/` so it turns to inverse video, then click on **Change**.

   You are now in the `vnmr` directory.

5. Click the mouse on `fidlib/` so it turns to inverse video, then click on **Change**.

   You are now in the `fidlib` directory.

6. Click the mouse on the `fid1d.fid` so it turns to inverse video, and then click on **Return** > **Load** > **Process** > **Transform**.

   A spectrum appears in the graphics window.

7. Click on **Next** > **Dscale**.

   A scale appears under the spectrum

8. Move the mouse arrow to about 4 ppm and click the *left* mouse button.

   The vertical line cursor moves to the point you clicked.

9. Move the mouse arrow to about 0.5 ppm and click the *right* button.

   A second vertical line appears at the point you clicked.

10. Click on **Expand**.

    An expansion of the region between the vertical cursors fills the window.

11. Move the mouse arrow above the group of peaks near 3.4 ppm and about halfway up the graphics window. Click the *center* button of the mouse.

    The vertical scale changes to bring the peaks to the location where you clicked the mouse arrow.

12. Reverse this process by moving the mouse down towards the baseline, directly under the same group of peaks, and click the center button again.

13. If your system is set up for a plotter, plot the spectrum by clicking on **Return** > **Plot** > **Plot** > **Scale** > **Params** > **Page**.

4.4 Permanent Menu

The Permanent menu is always available on the upper row of menu system. To make a choice, move the mouse cursor over the button label with the action desired and click (press down and release) the left mouse button. Unlike all other menus, the function keys on the keyboard can't be used to make selections on this menu. The following choices are standard on the Permanent menu.

Button	*Description*
Abort Acq	Abort (terminate) an experiment (acquisition) currently in progress.
Cancel Cmd	Cancel the currently active command, and all commands pending after that one, regardless of whether the commands were initiated through the keyboard, a mouse button, or by some other means.
GLIDE	Activates the *GLIDE* user interface window. After *GLIDE* is activated, clicking on the GLIDE button toggles the *GLIDE* user interface so it is alternately hidden (actually placed in the back of other windows) and displayed (brought to the front of other windows).
Main Menu	Display the Main menu on the lower row of buttons (page 66).
Help	Display the help screen for the currently active menu.
Flip	Alternately uncover and conceal the text window. Used when the graphics window covers the text window.

Button	*Description*
Resize	Changes the size of the graphics window. If the graphics window is small (the graphics window and the text window can be viewed at the same time), clicking on Resize enlarges the graphics window to cover most of the screen. Alternatively, if the graphics screen is large, clicking on Resize reduces it back to the default size. When the graphics window covers the text output window, the Flip button (above) is then used to alternately uncover and conceal the text window.
Acqi	Opens an acquisition window. If your system is not configured for acquisition, you will not see this button.

4.5 Main Menu

Of all of the menus, the most important is the Main menu, because it serves as a focal point from which all other menus can be reached. If you think of the menu system as a tree, the Main menu is the trunk from which all the other menus grow. Since the Main menu can be reached at all times by using the Main Menu button in the Permanent menu, you can very quickly get from any place in the menu system to any place else.

The choices in the Main menu enable you to display ten second-level menus, including the Secondary Main menu, which is an extension of the Main menu. Many of the lower menus return directly to Main menu after the button actions on the lower menu are completed. To make a choice on the Main menu and all lower menus, move the mouse cursor over the button label with the action desired and click (press down and release) the left mouse button.

The Main menu is activated by selecting Main Menu in the Permanent menu or by entering the command `menu('main')` in the input window.

Button	*Description*
Workspace	Display the Workspace menu (page 67) for selection of the experiment (workspace) to be used.
Setup	Display the Setup menu (page 67) to set up parameters for data acquisition.
Acquire	Display the Acquire menu (page 70) to initiate data acquisition using one of several modes.
Process	If a 1D experiment is active, display the 1D Data Processing menu (page 71) for processing data (weighting, Fourier transform). If a 2D experiment is active, display the 2D Data Processing menu (page 73) for processing data (weighting, Fourier transform).
Display	If a 1D experiment is active, display the 1D Data Display menu (page 77) for display of previously processed data. If a 2D experiment is active, display the 2D Data Display menu (page 79) for display of previously processed data.
Analyze	Display the Analyze menus page 81) for access to various spectral analysis tools, including spin simulation, deconvolution, spectral add/subtract, regression, and exponential analysis.
File	Display the Files Main menu (page 87) to retrieve or store data, edit files, etc.
More	Display the Secondary Main menu (page 91) for other (less common) choices, including writing a pulse sequence, opening a temporary UNIX shell, and exiting VNMR.

4.6 Workspace Menu

All data acquisition and data processing is done using a series of files known collectively as an *experiment*. Experiments have names `exp1` through `exp9`. Of these, all except `exp5` can be used for general-purpose experiments (`exp5` is used for the spectra add/subtract mode). At any one time, you are joined with (or connected to) a particular experiment, but you can create up to nine experiments and switch back and forth between experiments according to your needs.

Selecting Workspace from the Main menu displays the Workspace menu, which enables you to display the current list of experiments, switch to any experiment, and create or delete experiment files (`exp1` is created by default and cannot be deleted). You can also enter `menu('workspace')` to display the Workspace menu.

Button	*Description*
Library	Display in the text window the size, pulse sequence used, and text of existing experiments.
Exp 2, Exp 3,...	Join experiment `exp2`, `exp3`, ..., `exp9`.
Create New	Create a new experiment, using the first available number.
Delete	Delete an experiment, prompting for user input.

4.7 Setup Menus

Selecting Setup in the Main menu activates the Setup menu, which is used to set up a new NMR experiment. To complete the setup, additional menus can be displayed from the Setup menu to select the nucleus, solvent, and pulse sequence.

Setup Menu

The Setup menu is useful for setting up new experiments from scratch or modifying existing experiments, for example, switching from a “normal” 1D carbon experiment to an APT experiment. You can also enter `menu('setup')` to display the Setup menu.

Button	*Description*
H1,CDCl3	Set up a standard proton experiment with $CDCl_3$ as solvent.
C13,CDCl3	Set up a standard carbon experiment with $CDCl_3$ as solvent.
Nucleus,Solvent	Display the Nucleus Selection menu (page 68) to set up a standard experiment using menus to select nucleus and solvent.
Sequence	Display the 1D Pulse Sequence Setup menu (page 68) to select a sequence from a list of 1D and 2D pulse sequences.
App Mode	Display the Applications Mode menu (page 70).
Acquire	Display the Acquire menu (page 70).

Nucleus Selection Menu

The Nucleus Selection menu sets the value of the transmitter nucleus parameter `tn` using input from the user, then displays the Solvent Selection menu. The Nucleus Selection menu is activated by selecting the Nucleus,Solvent button in the Setup menu, by entering the command `setup`, or by entering `menu('nucleus')`.

Button	*Description*
H1	Set nucleus for ^{1}H.
H2	Set nucleus for ^{2}H.
C13	Set nucleus for ^{13}C.
N15	Set nucleus for ^{15}N.
F19	Set nucleus for ^{19}F.
P31	Set nucleus for ^{31}P.
Other	Shows prompt “Enter Nucleus of Interest:” and sets nucleus to that value.
Return	Display the Setup menu (page 67).

Solvent Selection Menu

The Solvent Selection menu sets the solvent to the value requested by the user, then returns the user to the Setup menu. This menu is typically activated by a selection of a nucleus on the Nucleus Selection menu or by entering `menu('solvent')`.

Button	*Description*
CDCl3	Set solvent for $CDCl_3$.
D2O	Set solvent for D_2O.
Benzene	Set solvent for benzene.
DMSO	Set solvent for DMSO.
Acetone	Set solvent for acetone.
Other	Shows prompt “Enter Solvent:” and sets solvent to that value.
Return	Display the Setup menu (page 67).

1D Pulse Sequence Setup Menu

The 1D Pulse Sequence Setup menu provides setups for five 1D experiments and access to menus for 2D and additional 1D experiments. This menu is activated by clicking on the Sequence button in the Setup menu or by `menu('psgset')`.

Button	*Description*
APT	Set up an Attached Proton Test pulse sequence for CH_n multiplet selection.
DEPT	Set up a DEPT pulse sequence for CH_n multiplet selection, spectrum editing, and signal enhancement.
INEPT	Set up an INEPT pulse sequence for CH_n multiplet selection and signal enhancement (this sequence not supplied with the *GEMINI 2000*).

Button	*Description*
BINOM	Set up a Binomial Water Suppression pulse sequence (this sequence not supplied with the *MERCURY-VX*, *MERCURY*, or *GEMINI 2000*).
S2PUL	Set up a S2PUL pulse sequence for the standard two-pulse experiment.
More 1D	Display the 1D Pulse Sequence Setup Secondary menu (below).
2D	Display the 2D Pulse Sequence Setup menu (page 69).
Return	Display the Setup menu (page 67).

1D Pulse Sequence Setup Secondary Menu

The 1D Pulse Sequence Setup Secondary menu provides setups for three more 1D experiments. This menu is activated by clicking on the More 1D button in the 1D Pulse Sequence Setup menu or by entering `menu('psgset1')`.

Button	*Description*
D2PUL	Set up a standard decoupler pulse sequence.
SSECHO	Set up a solid-state echo pulse sequence (only applicable on systems with the solid-state NMR accessory installed).
XPOLAR	Set up a cross-polarization pulse sequence for solids (only applicable on systems with the solid-state NMR accessory installed).
More 1D	Display the 1D Pulse Sequence Setup menu (above).
2D	Display the 2D Pulse Sequence Setup menu (page 69).
Return	Display the Setup menu (page 67).

2D Pulse Sequence Setup Menu

The 2D Pulse Sequence Setup menu provides setups for five 2D experiments and access to menus for 1D and additional 2D experiments. This menu is activated by clicking on the 2D button in the 1D Pulse Sequence Setup menu or by entering `menu('psgset2')`.

Button	*Description*
COSY	Set up a homonuclear correlation pulse sequence, absolute value.
COSYPS	Set up a phase-sensitive, pure absorption COSY pulse sequence.
HETCOR	Set up a heteronuclear correlation pulse sequence.
NOESY	Set up a NOE 2D correlation pulse sequence.
ROESY	Set up a rotating frame NOE 2D correlation pulse sequence.
1D	Display the 1D Pulse Sequence Setup menu (page 68).
More 2D	Display the 2D Pulse Sequence Setup Secondary menu (below).
Return	Display the Setup menu (page 67).

2D Pulse Sequence Setup Secondary Menu

The 2D Pulse Sequence Setup Secondary menu provides setups for five more 2D experiments and access to menus for 1D and additional 2D experiments. This menu is activated by clicking on the More 2D button in the 2D Pulse Sequence Setup menu or by entering `menu('psgset3')`.

Button	*Description*
DQCOSY	Set up a COSY with double-quantum filtered pulse sequence.
HET2DJ	Set up a heteronuclear J-resolved 2D pulse sequence.
INADQT	Set up a carbon-carbon connectivity 2D (2D INADEQUATE) pulse sequence (this sequence not supplied with the *GEMINI 2000*).
HOM2DJ	Set up a homonuclear J-resolved 2D pulse sequence.
TOCSY	Set up a total correlation 2D pulse sequence (this sequence not supplied with the *GEMINI 2000*).
1D	Display the 1D Pulse Sequence Setup menu (page 68).
More 2D	Display the 2D Pulse Sequence Setup menu (above).
Return	Display the Setup menu (page 67).

Applications Mode Menu

Different applications modes give access to extra or different macros and menus if they have been installed. The Applications Mode menu is entered by selecting App Mode in the Setup menu, or by entering the command `menu('appmode')`.

Button	*Description*
Standard	Set parameter `appmode` to `'standard'` and set system lookup paths for `maclib`, `menulib`, and `help` to the standard directories `/vnmr/maclib`, `/vnmr/menulib`, and `/vnmr/help`.
Imaging	Set parameter `appmode` to `'imaging'` and set system lookup paths for `maclib`, `menulib`, and `help` to look in the imaging directories defined by the parameters `systemmenulibpath` and `syshelppath` before looking in the standard system directories.
Return	Display the Setup menu (page 67).

4.8 Acquire Menu

Data acquisition in a variety of modes can be initiated with the Acquire menu. This menu is typically entered by selecting the Acquire button in the Main menu, by selecting the Acquire button in the Setup menu, or by entering the command `menu('acquire')`.

Button	*Description*
Show Time	Display time that current experiment takes if acquisition is started with existing parameters.
Go	Begin an acquisition with no subsequent data processing.
Go, Wft	Begin an acquisition, and weight and Fourier transform the FID automatically when acquisition is complete.

Button	*Description*
Go, Periodic Wft	Begin an acquisition, and weight and Fourier transform the FID periodically, after each `bs` transients are completed.
Automatic	Begin an acquisition, and process data according to the parameters `wbs`, `wnt`, and `wexp`.

4.9 Processing Menus

Two different data processing menus are possible, depending upon whether a 1D or 2D experiment is active.

1D Data Processing Menu

The 1D Data Processing menu is typically entered by selecting the Process button in the Main menu when a 1D experiment is active, by selecting the Reprocess button in the 1D Data Display menu, or by entering the command `menu('process_1D')`.

Button	*Description*
Display FID	Display the Interactive 1D FID Display menu (below).
Select Params	Display the 1D Processing Parameter Setup menu (page 72).
Adj Weighting	Display the Interactive Weighting menu (page 72).
Transform	Perform non-weighted Fourier transformation of all spectra, and then display the Interactive 1D Spectrum Display menu (page 71).
Weight, Transform	Perform weighted Fourier transformation of all spectra, then display the Interactive 1D Spectrum Display menu (page 73).

Interactive 1D FID Display Menu—df Program

The Interactive 1D FID Display menu (part of the `df` program) is typically entered by selecting the Display FID button in the 1D Data Processing menu or by entering the command `df<(index)>`. If called with an `index` number as an argument, the desired FID number in a multi-FID experiment is selected; otherwise, the current index is used.

Button	*Description*
Box –OR– Cursor	If labeled Box, select two cursors (go to the box mode). If labeled Cursor, select one cursor (go to the cursor mode).
Imaginary –OR– Zero Imag –OR– No Imag	If labeled Imaginary, display the imaginary FID. If labeled Zero Imag, display the imaginary FID as all zero. If labeled No Imag, remove the imaginary FID display.
Expand –OR– Full	If labeled Expand, expand to area between cursors (box mode). If labeled Full, display full area (cursor mode).
sf wf	Adjust the start and width of the displayed FID.
Dscale	Toggle the display of a time scale.
Phase	Enter the interactive phasing mode.
Return	Return to last menu active before entering the `df` program.

1D Processing Parameter Setup Menu

Parameters can be set up to the standard values with one of the buttons on the 1D Processing Parameter Setup menu or they can be typed in and observed (e.g., type `fn=8000`). After parameter selection, return to the 1D Data Processing menu with the Return button. The 1D Processing Parameter Setup menu is activated by selecting Select Params in the 1D Data Processing menu or by entering the command `menu('procpar_1D')`.

Button	*Description*
No WT	Clear all weighting parameters.
Resolve	Select default resolution enhancement parameters.
Broaden	Select standard line broadening parameters.
->AV –OR– ->PH	If labeled ->AV, switch to the absolute-value mode. If labeled ->PH, switch to the phase-sensitive mode. The value of the parameter `dmg` determines the button label.
FN: Small	Select Fourier number for quick transform.
Normal	Select Fourier number for normal size transform.
Large	Select Fourier number for large transform with zero filling.
Return	Display the 1D Data Processing menu (page 71).

Interactive Weighting Menu—wti Program

The Interactive Weighting menu (part of the `wti` program) is typically entered by selecting the Adj Weighting button in the 1D Data Processing menu, in the 2D Data Processing menu, or in the 2D Interferogram Processing menu, or by entering the command `wti<(index)>`. If called with an `index` number as an argument, the desired FID number in a multi-FID experiment is selected; otherwise, the current index is used. This menu is not user-programmable.

Button	*Description*
next fid	Increment FID/interferogram index.
lb	Select line broadening or exponential weighting. Negative gives resolution enhancement.
sb	Select sinebell constant. Negative gives squared sinebell.
sbs	Select sinebell shift constant (only if sinebell is active).
gf	Select Gaussian time constant.
gfs	Select Gaussian time constant shift (only if Gaussian time constant is active).
awc	Select additive weighting constant.
Return	Return to last menu active before entering the `wti` program.

Interactive 1D Spectrum Display Menu—ds Program

The Interactive 1D Spectrum Display menu (part of the `ds` program) is typically entered by selecting the Transform button or the Weight,Transform button in the 1D Data Processing menu, or by entering the `menu('ds_1')` or `ds` command.

Button	*Description*
Box –OR– Cursor	If labeled Box, select two cursors (go to box mode). If labeled Cursor, select one cursor (go to cursor mode).
No Integral –OR– Full Integral –OR– Part Integral	If labeled No Integral, hides integral display. If labeled Full Integral, display all integral regions. If labeled Part Integral, display every other region.
Expand –OR– Full	If labeled Expand, expand to area between cursors (box mode). If labeled Full, display full area (cursor mode).
sp wp	Adjust the start and width of the displayed spectrum.
Mark	Mark cursor position (in cursor mode) or region (box mode).
Phase	Enter the interactive phasing mode.
Th	Interactively adjust the horizontal threshold.
Resets	Interactively define or remove integral reset points.
Dscale	Toggle on and off the display of a scale below the spectrum.
Lvl/Tlt	Interactively adjust `lvl` and `tlt` parameters.
Set Int	Set integral scaling.
Return	Return to last menu active before entering the `ds` program.

2D Data Processing Menu

The 2D Data Processing menu is activated by selecting the Process button in the Main menu when a 2D experiment is active or by selecting the Reprocess button in the 2D Display menu. It can also be entered through the command `menu('process_2D')`.

Button	*Description*
Select Params	Display the 2D Processing Parameter Setup menu (below).
Adj Weighting	Display the Interactive Weighting menu (page 72).
Phase F2	Perform a 1D FT of first FID to allow phasing along f_2 dimension (only active in phase-sensitive mode).
Transform F2	Perform a full set of transforms of the FIDs along the t_2 axis and display the Interactive 2D Color Map Display Main menu (page 74). Any currently active weighting functions are used.
Full Transform	Perform a full set of transforms, first along t_2, then along t_1, using any currently active weighting functions. At the end of processing, display the Interactive 2D Color Map Display Main menu (page 74).

2D Processing Parameter Setup Menu

Parameters can be set up to the standard values with one of the buttons on the 2D Processing Parameter Setup menu or they can be typed in and observed (e.g., type `fn=512`). After parameter selection, return to the 2D Data Processing menu with the Return button.

The 2D Processing Parameter Setup menu is activated by selecting the Select Params button in the 2D Data Processing menu or by entering `menu('procpar_2D')`.

Button	*Description*
No WT	Clear all weighting parameters.
Sinebell	Select sinebell weighting over the whole FID length.
Pseudo	Select “pseudo-echo” weighting.
->AV –OR– ->PH	If labeled AV, switch to the absolute-value mode. If labeled PH, switch to the phase-sensitive mode. The value of the parameter `dmg` determines the button label.
FN: Small	Select Fourier number for quick transform.
Normal	Select Fourier number for normal size transform.
Large	Select Fourier number for large transform with zero filling.
Return	Display the 2D Data Processing menu (above).

2D Interferogram Processing Menu

The 2D Interferogram Processing menu is activated by selecting the Transform F2 button in the 2D Data Processing menu or by entering `menu('process_IF')`.

Button	*Description*
Color Map	Display the Interactive 2D Color Map Display Main menu (below).
Adj Weighting	Display the Interactive Weighting menu (page 72).
F1 Transform	Perform second Fourier transformation along f_1.
Reprocess	Display the 2D Data Processing menu (page 73) to repeat first Fourier transformation.

Interactive 2D Color Map Display Main Menu—dconi Program

The Interactive 2D Color Map Display Main menu (part of the `dconi` program) is activated by selecting Transform F2 or Full Transform in the 2D Data Processing menu, by selecting Color Map in the 2D Interferogram Processing menu, or by entering the command `dconi`.

Button	*Description*
Box –OR– Cursor	If labeled Box, select two pairs of cursors (box mode). If labeled Cursor, select one pair of cursors (cursor mode).
Trace	Select trace display mode.
Proj	Display the Interactive 2D Display Projection menu (page 75).
Expand –OR– Full	If labeled Expand, expand to area between cursors (box mode). If labeled Full, display full area (cursor mode).
Redraw	Repeat the last 2D or image display with current parameters.
Plot	Plot current trace.
Peak	Display the Interactive 2D Peak Picking Main menu (page 75).
Return	Return to previous menu.

Interactive 2D Display Projection Menu—dconi Program

The Interactive 2D Display Projection menu (part of the `dconi` program) is activated by selecting the Proj button in the Interactive 2D Color Map Display Main menu.

Button	*Description*
Hproj (max)	Horizontal projection of the maximum intensity at each frequency.
Hproj (sum)	Horizontal projection of the summed intensity at each frequency.
Vproj (max)	Vertical projection of the maximum intensity at each frequency.
Vproj (sum)	Vertical projection of the summed intensity at each frequency.
Plot	Plot current projection.
Cancel	Display the Interactive 2D Color Map Display Main menu (page 74).

Interactive 2D Peak Picking Main Menu—ll2d Program

The Interactive 2D Peak Picking Main menu (part of the `ll2d` program) is activated by selecting the Peak button in the Interactive 2D Color Map Display Main menu.

Button	*Description*
Auto	Display the 2D Peak Picking Automatic menu (next)
Edit	Display the 2D Peak Picking Edit menu (page 76)
File	Display the 2D Peak Picking File menu (page 76)
Display	Display the 2D Peak Picking Display menu (page 76)
Return	Display the Interactive 2D Color Map Display Main menu (page 74).

2D Peak Picking Automatic Menu—ll2d Program

The 2D Peak Picking Automatic menu (part of the `ll2d` program) is activated by selecting the Auto button in the Interactive 2D Peak Picking Main menu.

Button	*Description*
Box –OR– Cursor	If labeled Box, select two pairs of cursors (box mode). If labeled Cursor, select one pair of cursors (cursor mode).
Peak	Automatically pick peaks.
Volume	Automatically determine peak bounds and calculate volumes.
Expand –OR– Full	If labeled Expand, expand to area between cursors (box mode). If labeled Full, display full area (cursor mode).
Both	Pick peaks and calculate volumes.
Adjust	Adjust peak bounds so that none overlap.
Reset	Delete all peaks in the peak table.
Return	Display the Interactive 2D Peak Picking Main menu (page 75).

2D Peak Picking Edit Menu—ll2d Program

The 2D Peak Picking Edit menu (part of the `ll2d` program) is activated by selecting the Edit button in the Interactive 2D Peak Picking Main menu.

Button	*Description*
Box –OR– Cursor	If labeled Box, select two pairs of cursors (box mode). If labeled Cursor, select one pair of cursors (cursor mode).
Mark	Mark peak (cursor mode) or volume (box mode) at current cursor location(s).
Unmark	Delete peak (cursor mode) or volume (box mode) at current cursor location(s)
Expand –OR– Full	If labeled Expand, expand to area between cursors (box mode). If labeled Full, display full area (cursor mode).
Clear	Delete peaks and volumes of peaks in the current display area.
Combine	Combine peaks into a single peak.
Label	Prompt for and label peak (cursor mode) or peaks (box mode) with 15-character label.
Comment	Prompt for and label peak (cursor mode) or peaks (box mode) with 80-character comment.
Info	Print information to text window about peak nearest the cursor.
Set Int	Set volume scaling.
Return	Display the Interactive 2D Peak Picking Main menu (page 75).

2D Peak Picking File Menu—ll2d Program

The 2D Peak Picking File menu (part of the `ll2d` program) is activated by selecting the File button in the Interactive 2D Peak Picking Main menu.

Button	*Description*
Read	Read in a binary peak file
Read Text	Read in a text peak file.
Write Text	Write out a text peak file.
Backup File	Prompt for a filename and copy current binary peak file to that file.
Return	Display the Interactive 2D Peak Picking Main menu (page 75).

2D Peak Picking Display Menu—ll2d Program

The 2D Peak Picking Display menu (part of the `ll2d` program) is activated by selecting the Display button in the Interactive 2D Peak Picking Main menu.

Button	*Description*
Sh Pk–OR– Hd Pk	If labeled Sh Pk, show a “+” at the location of each peak. If labeled Hd Pk, hide (do not show) a “+” at each peak.
Sh Num –OR– Hd Num	If labeled Sh Num, show a peak number next to each peak. If labeled Hd Num, hide (do not show) peak numbers.
Sh Box –OR– Hd Box	If labeled Sh Box, show a box with the area integrated to get the volume of the peak. If labeled Hd Pk, hide this box.

Button	*Description*
Sh Lbl–OR– Hd Lbl	If labeled Sh Lbl, show a peak label next to each peak. If labeled Hd Lbl, hide (do not show) peak labels.
Sh All	Show “+”, number, box, and label for all peaks.
Hd All	Hide (do not show) “+”, number, box, and label for all peaks.
Return	Display the Interactive 2D Peak Picking Main menu (page 75).

4.10 Display Menus

Two different menus for display of data are provided. The menu displayed depends on whether a 1D or 2D experiment is active.

1D Data Display Menu

The 1D Data Display menu is activated by selecting the Display button in the Main menu while a 1D experiment is active or by entering the command `menu('display_1D')`.

Button	*Description*
View	Display normal 1D spectrum and scale. No interactive adjustment is allowed.
Interactive	Display normal 1D spectrum and allow for interactive adjustment.
Massage	Display the 1D Data Manipulation menu (next).
Size	Display the 1D Display Size Selection menu (page 78).
Reprocess	Display the 1D Data Processing menu (page 71).
Plot	Display the 1D Plotting menu (page 78).
More	Display the 1D Data Display Secondary menu (page 78).

1D Data Manipulation Menu

The 1D Data Manipulation menu is activated by selecting the Massage button in the 1D Data Display menu or by entering the command `menu('massage_1D')`.

Button	*Description*
DC	Drift correct and display the selected spectrum.
Region	Automatic selection of peak regions in the selected spectrum and display the result.
BC	Perform a fifth-order baseline correction using the current integral reset points to determine peak regions. Display the resulting spectrum.
Autophase	Perform automatic calculation of the spectral phase parameters, then display the result.
Adj VS	Adjust vertical scale, then display the spectrum.
Adj IS	Adjust integral scale, then display the spectrum.
Adj WP	Adjust width of plot, then display the spectrum.
Return	Display the 1D Data Display menu (page 77).

1D Display Size Selection Menu

The 1D Display Size Selection menu is activated by selecting the Size button in the 1D Data Display menu or by entering the command `menu('size_1D')`.

Button	*Description*
Left	Set display for left half of the screen/page.
Center	Set display for center of the screen/page.
Right	Set display for right half of the screen/page.
Full Screen	Set display for full screen/page.
Return	Display the 1D Data Display menu (page 77).

1D Plotting Menu

The 1D Plotting menu is activated by selecting the Plot button in the 1D Data Display menu or by entering the command `menu('plot_1D')`.

Button	*Description*
Plot	Plot the selected spectrum. If the integral is currently displayed, plot the integral as well.
Scale	Plot an axis below the spectrum.
HP Params	Plot parameters below the spectrum in a special format when the plotting device is a Hewlett-Packard plotter.
Params	Print parameters in the left upper corner of paper using “English-language” format.
All Params	Print parameters in the left upper corner of paper using “mnemonic” format.
Peaks	Plot peak frequencies above peaks.
Page	Plot out the currently buffered plot and change paper.
Return	Display the 1D Data Display menu (page 77).

1D Data Display Secondary Menu

The 1D Data Display Secondary menu is activated by selecting the More button in the 1D Data Display menu or by entering the command `menu('display_1D_2')`.

Button	*Description*
Lines	Display list of spectral line frequencies and amplitudes. The parameter `th` is used as the listing threshold.
Integrals	Display list of integral intensities using the current set of integral reset points. If parameter `intmod='partial'`, every other integral is listed. If `intmod='full'` or `intmod='off'`, every integral is listed. The `ins` parameter acts as a divisor for this listing of integral amplitudes.
Dssh	Display spectra horizontally with a scale under first spectrum.
Dssa	Display spectra with automatic adjustment of the parameters `ho` and `vo`. Display a scale under the first spectrum.

Button	*Description*
AV –OR– PH	If labeled AV, switch to the absolute-value mode. If labeled PH, switch to the phase-sensitive mode. The value of the parameter `dmg` determines the button label.
Reference	Reference the spectrum so as to set the cursor position to zero on the chemical shift scale.
Return	Return to the 1D Data Display menu (page 77).

2D Data Display Menu

The 2D Data Display menu is activated by selecting the Display button in the Main menu while a 2D experiment is active or by entering the command `menu('display_2D')`.

Button	*Description*
Color Map	Display normal 2D contour display (color image or map) and allow for interactive adjustment.
Contour	Display a true 2D contour display, comparable to plotter output (this mode is slower than a simple color map).
Image	Display grayscale image and allow interactive adjustment.
Size	Display the 2D Display Size Selection menu (below).
Massage	Display the 2D Data Manipulation menu (page 79).
Reprocess	Display the 2D Data Processing menu (page 73).
Plot	Display the 2D Plotting menu (page 80).
More	Display the 2D Data Display Secondary menu (page 80).

2D Display Size Selection Menu

The 2D Display Size Selection menu is activated by selecting the Size button in the 2D Data Display menu or by entering the command `menu('size_2D')`.

Button	*Description*
Left	Set display for left half of the screen/page.
Center	Set display for center of the screen/page.
Right	Set display for right half of the screen/page.
Full Screen	Set display for full screen/page.
Full with Traces	Set display to use most of the screen/page, but leaving sufficient room at the top and left for traces and projections.
Return	Display the 2D Data Display menu (above).

2D Data Manipulation Menu

The 2D Data Manipulation menu is activated by selecting the Massage button in the 2D Data Display menu or by entering the command `menu('massage_2D')`.

Button	*Description*
DC(f2)	Drift correct the 2D data set along the f_2 axis.

Button	*Description*
DC(f1)	Drift correct the 2D data set along the f_1 axis.
Foldt	Perform a trigonal symmetrization (for COSY, COSYPS, COSY3, DQCOSY).
Foldj	Perform a symmetrization in J-resolved 2D spectra (for HET2DJ, HOM2DJ after rotation).
Foldcc	Perform a symmetrization in 2D INADEQUATE (for CCC2D, CCC2DQ).
Rotate	Rotate spectral data by 45° (for HOM2DJ).
Normalize	Normalize vertical scale for 2D display.
Return	Display the 2D Data Display menu (page 79).

2D Plotting Menu

The 2D Plotting menu is activated by selecting the Plot button in the 2D Data Display menu or by entering the command `menu('plot_2D')`.

Button	*Description*
All Contours	Calculate a contour plot of the current data.
Pos. Only	Calculate a contour plot of the positive current data.
Image	Print a grayscale image on a dot matrix printer (LaserJet, QuietJet, or InkJet—does not work on pen plotters).
All Params	Print parameters on printer.
Params	Plot parameters in the left upper corner of the paper.
Page	Plot out the currently buffered plot and change paper.
Return	Display the 2D Data Display menu (page 79).

2D Data Display Secondary Menu

The 2D Data Display Secondary menu is activated by selecting the More button in the 2D Display menu or by entering the command `menu('display_2D_2')`.

Button	*Description*
Stacked Plot	Display data stacked and whitewashed and allow for interactive adjustment.
F1 Mode –OR– F2 Mode	If labeled F1 Mode, select the f_1 axis to be horizontal. If labeled F2 Mode, select the f_2 axis to be horizontal.
AV –OR– PH	If labeled AV, switch to the absolute-value mode. If labeled PH, switch to the phase-sensitive mode. The value of the parameter `dmg` determines the button label.
Reference	Reference in both dimensions, set cursor positions to zero chemical shift on the scale.
Analyze	Allow 2D analysis, including line listing and automatic COSY correlation map.
Return	Return to the 2D Data Display menu (page 79).

4.11 Analyze Menus

A variety of data analysis tools are provided in VNMR, including exponential analysis, automatic DEPT and COSY analysis, spectral add/subtract, spin simulation, deconvolution, and regression analysis.

Analyze Menu

The Analyze menu is activated by selecting the Analyze button in the Main menu or by entering the command `menu('analyze')`.

Button	*Description*
Exponential	Display the Exponential Analysis menu (below).
DEPT	Display the Automatic DEPT Analysis menu (page 81) for full spectral editing capabilities.
COSY	Display the Automatic COSY Analysis menu (page 82).
Add/Sub	Display the Add/Subtract menu (page 82).
Simulation	Display the Spin Simulation Main menu (page 83).
Deconvolution	Display the Deconvolution menu (page 85).
Regrs	Display the Regression 1 menu (page 86) and run the command `expl('regression')`.

Exponential Analysis Menu

The Exponential Analysis menu is activated by selecting the Exponential button in the Analyze menu or by entering the command `menu('t1t2anal')`.

Button	*Description*
T1 Proc	Weight, Fourier transform, phase each FID in a T_1 data set.
T1 Analysis	Perform an exponential least-squares analysis on each peak in the spectrum to determine its T_1 value.
T2 Proc	Weight, Fourier transform, phase each FID in a T_2 data set.
T2 Analysis	Perform an exponential least-squares analysis on each peak in the spectrum to determine its T_2 value.
Plot	Produce a horizontal stacked plot of the spectra used in the exponential analysis.
Print	Print the information from the exponential least-squares analysis.
Return	Display the Main menu (page 66).

Automatic DEPT Analysis Menu

The Automatic DEPT Analysis menu is activated by selecting the DEPT button in the Analyze menu or by entering the command `menu('dept')`.

Button	*Description*
Process	Weight, Fourier transform, phase each FID in the data set.
Display	Display the current spectra (edited or unedited).

Button	*Description*
Plot	Plot the current spectra (edited or unedited).
Edit	Edit processed spectra to obtain separation of CH, CH_2, and CH_3 peaks.
Printout	Print editing information contained in the `dept.out` text file in the current experiment directory.
Full Analysis	Process spectra, plot unedited spectra, edit spectra, plot edited spectra, and print editing information (each action within this selection can be accomplished individually by buttons 1 to 5).
Return	Display the Main menu (page 66).

Automatic COSY Analysis Menu

The Automatic COSY Analysis menu is activated by selecting COSY in the Analyze menu or by entering the command `menu('auto2D')`.

Button	*Description*
2D Line List	Perform a 2D line listing and display the peaks with the dconi program, if `dconi` was active prior to selecting this button.
Find Correlations	Perform an automatic 2D COSY analysis. The analysis uses the information from the last 2D line listing, which must be performed first. Display the result on the screen.
Plot Correlations	Perform an automatic 2D COSY analysis, using the information from the last 2D line listing, and plot the results on the plotter. A contour plot is not plotted by this button, but the 2D Plotting menu (page 80) will be displayed to allow a selection of additional items to be added to the plot, typically just a contour plot.
Redisplay	Display a normal 2D contour map and allow for interactive adjustment.
Return	Display the 2D Data Display menu (page 79).

Add/Subtract Menu

The Add/Subtract menu is activated by selecting Add/Sub in the Analyze menu or by entering the command `menu('addsub')`.

Button	*Description*
Clear	Clear the add/subtract experiment (`exp5`).
Interactive Mode	Display the Interactive Add/Subtract menu (below), taking the currently active spectrum as one input and a spectrum that has been previously placed into the add/subtract experiment as the second input.
Add Spectrum	Non-interactive addition of the current spectrum into the add/subtract experiment.
Subtract	Non-interactive subtraction of the current spectrum into the add/subtract experiment.
Minimum	Non-interactive combination of the minimum of the current spectrum and the spectrum in the add/subtract experiment.

Interactive Add/Subtract Menu—addi Program

The Interactive Add/Subtract menu (part of the `addi` program) is typically entered by clicking on the Interactive Mode button in the Add/Subtract menu, by selecting the Add/Sub button in the Deconvolution menu, or by entering the command `addi`.

Button	*Description*
Box –OR– Cursor	If labeled Box, go to the box mode with two cursors. If labeled Cursor, go to the cursor mode with one cursor.
Select	Select the current, add/sub, or result spectrum as active.
Expand –OR– Full	If labeled Expand, expand area between cursors (box mode). If labeled Full, display full area (cursor mode).
sp wp	Adjust the start and width of the active spectrum.
sub –OR– min –OR– add	If labeled sub, select the result spectrum to be the difference between the current and the add/sub spectra. If labeled min, select the result spectrum to be a minimum intensity of either the current or the add/sub spectra. If labeled add, select the result spectrum to be a sum of the current and the add/sub spectra.
save	Save the result spectrum in the add/sub experiment and return to the last menu.
Return	Return to the last menu without saving the result.

Spin Simulation Main Menu

The Spin Simulation Main menu is the first of six menus covering almost the entire analysis of spin simulation. The Spin Simulation Main menu is activated by selecting Simulation in the Analyze menu or by entering the command `menu('spins')`.

Button	*Description*
Spin System	Display the Spin Simulation First Definition menu (below) to select a spin system.
Show Params	Display parameters and allow for changes.
Set Params	Set spin simulation parameters (`sminf`, `smaxf`, `slw`, `svs`, and `niter`) from the current display.
Simulate	Perform a spin simulation using the current parameters.
Original	Fourier transform and display the experimental spectrum.
Next	Display the Spin Simulation Secondary menu (page 84).

Spin Simulation First Definition Menu

The Spin Simulation First Definition menu is activated by selecting the Spin System button in the Spin Simulation Main menu or by entering `menu('spins1')`.

Button	*Description*
AB	Select two-spin system AB.
ABC	Select three-spin system ABC.
A2B	Select three-spin system A2B.

Button	*Description*
ABCD	Select four-spin system ABCD.
A2BC	Select four-spin system A2BC.
A3B	Select four-spin system A3B.
Other	Display Spin Simulation Second Definition menu (below).
Return	Display the Spin Simulation Main menu (above).

Spin Simulation Second Definition Menu

The Spin Simulation Second Definition menu is activated by selecting the Other button in the Spin Simulation First Definition menu or by entering `menu('spins1_2')`.

Button	*Description*
ABCDE	Select five-spin system ABCDE.
A2BCD	Select five-spin system A2BCD.
A3BC	Select five-spin system A3BC.
A2B2C	Select five-spin system A2B2C.
A3B2	Select five-spin system A3B2.
A3B2C	Select six-spin system A3B2C.
Other	Display Spin Simulation Third Definition menu (below).
Return	Display the Spin Simulation Main menu (page 83).

Spin Simulation Third Definition Menu

The Spin Simulation Third Definition menu is activated by selecting the Other button in the Spin Simulation Second Definition menu or by entering `menu('spins1_3')`.

Button	*Description*
AX	Select spin system AX.
AXY	Select spin system AXY.
AX2	Select spin system AX2.
AXYZ	Select spin system AXYZ.
AX2Y	Select spin system AX2Y.
AX3	Select spin system AX3.
Other	Show prompt "`Spin System?`" and set system to that value.
Return	Display the Spin Simulation Main menu (page 83).

Spin Simulation Secondary Menu

The Spin Simulation Secondary menu is activated by selecting the Next button in the Spin Simulation Main menu or by entering `menu('spins2')`.

Button	*Description*
list	Display listing of last spin simulation.

Button	*Description*
params	Display parameters and allow for changes.
assign	Run the `dla` program and display the Spin Simulation Line Assignment menu (page 85).
display	Calculate and display the simulated spectrum.
iterate	Perform an iterative optimization and display the resulting spectrum.
observe	Fourier transform and display the experimental spectrum.
Return	Display the Spin Simulation Main menu (page 83).
Main	Display the Main menu (page 66).

Spin Simulation Line Assignment Menu

The Spin Simulation Line Assignment menu is activated by selecting the Assign button in the Spin Simulation Secondary menu or by entering `menu('spins_assign')`.

Button	*Description*
ll	Perform a line listing on the current spectrum.
use ll	Use the last line listing as a reference for the line assignments.
use fitspec	Use last deconvolution as a reference for the line assignments.
auto assign	Run the `assign` macro to assign lines for iterative optimization from a `dll` or `nll` listing.
iterate	Perform iterative optimization and display resulting spectrum.
Return	Display the Spin Simulation Secondary menu (above).
Main	Display the Main menu (page 66).

Deconvolution Menu

The Deconvolution menu is activated by selecting the Deconvolution button in the Analyze menu or by entering `menu('fitspec')`.

Button	*Description*
Use Line List	Perform line listing on the current spectrum (observed or calculated, whichever was displayed last) and use the listing as a starting point for a deconvolution. `slw` is set to the measured width of the tallest line in the displayed spectrum.
Use Mark	Use file `mark1d.out` (created by the “mark” option while interactively displaying a spectrum) as the starting point for a deconvolution. If mark done with a single cursor, the information is used to initialize the frequencies and intensities only, with `slw` set to the measured width of the tallest line in the displayed spectrum. If mark was done with two cursors, the average frequency of the cursors is the peak frequency, and the difference is the line width, thus allowing different starting line widths for different lines in the spectrum.
Fit	Fit the current spectrum using the current starting parameters (usually set with 1 or 2). The original spectrum is first saved in `exp5` for possible later use in add/subtract operations.
Results	Display the numeric results of the last fit.
Show Fit	Display the simulated spectrum.

Button	*Description*
Plot	Plot the original spectrum, the simulated spectrum, the individual components, and the numeric results.
Add/Sub	Change to the Interactive Add/Subtract menu (page 83) and display the original and simulated spectra.

Regression 1 Menu

The Regression 1 menu is the first of three menus for performing regression analysis. To display the Regression 1 menu with a display of data in the `regression.inp` file, click the Analyze button in the Main menu, then click on the Regrs button. This menu can also be activated by entering `menu('regression1')`.

Button	*Description*
x-linear	Show the displayed data points against a linear *x*-axis scale.
x-square	Show the displayed data points against a squared *x*-axis scale.
x-log	Show the displayed data points against a logarithmic *x*-axis scale.
dp-linear	Fit a straight line to the data points and display.
dp-quad	Fit a quadratic curve to the data points and display.
dp-exp	Fit a exponential curve to the data points and display.
Next	Display the Regression 2 menu (below).
Rt	Display the Analyze menu (page 81).

Regression 2 Menu

The Regression 2 menu is activated by selecting the Next button in the Regression 1 menu or by entering `menu('regression2')`.

Button	*Description*
y-linear	Show the displayed data points against a linear *y*-axis scale.
y-square	Show the displayed data points against a squared *y*-axis scale.
y-log	Show the displayed data points against a logarithmic *y*-axis scale.
dp-linear	Fit a straight line to the data points and display.
dp-quad	Fit a quadratic curve to the data points and display.
dp-exp	Fit a exponential curve to the data points and display.
Next	Display the Regression 3 menu (below).
Rt	Display the Regression 1 menu (above).

Regression 3 Menu

The Regression 3 menu is activated by selecting the Next button in the Regression 2 menu or by entering `menu('regression3')`.

Button	*Description*
dp-linear	Fit a straight line to the data points and display.

Button	*Description*
dp-quad	Fit a quadratic curve to the data points and display.
dp-cubic	Fit a cubic curve to the data points and display.
dp-exp	Fit an exponential curve to the data points and display.
plot	Plot the displayed data and curves.
dp output	Display the results of the analysis in the text window.
Return	Display the Regression 1 menu (page 86).

4.12 File Menus

A series of eight menus for handling files are accessible using th File button in the Main menu or by entering the `files` command. The following applies to all `files` menus:

- To make a choice on a menu, move the mouse cursor over the button and click (press and release the button) with the left mouse button.
- To select or mark a file in the list of displayed file names, move the mouse cursor over the desired filename and use the left mouse button to click on the name so that the name changes to reverse video. To deselect a filename, click on it again. File names with a slash "`/`" after the name are directories.
- Some operations permit more than one filename to be selected. To select additional file names, simply click on them.
- If you do not select a file name when required, VNMR displays a prompt requesting the entry of the file name in the input window.

Files Main Menu

The Files Main menu is activated by selecting the File button in the Main menu or by entering the command `files`.

Button	*Description*
Set Directory	If a directory has been selected in the `files` display (directories have a "`/`" following their names), that becomes the new current directory. If you haven't selected a directory, the Directory menu (below) is displayed for you to select a new current directory.
File Info	Display Files Information menu (page 89) to list the files in the current directory, sorted by size or data of modification.
Tape	Display Files Tape menu (page 89) to read and write tapes. (See Chapter 10, "Storing, Retrieving, and Moving Data," for other types of tapes.)
Load	First mark one entry in the `files` display and then click on this button. If you have selected an entry that has Varian NMR data, including data from a Gemini, VXR, or XL system, that parameter set and data is loaded into the current experiment. If the entry is a parameter set, the parameters are loaded.
Data	Display Files Data menu (page 90) with choices for accessing NMR data and related files.
Delete	First mark one or more files and/or directories in the `files` display (directories have a "`/`" following their names) and then click on this button. Each entry you have marked, including subdirectories and their contents, is deleted.

Button	*Description*
More	Display the Files Secondary menu (page 90) for additional options.
Return	Display the Main menu (page 66).

Directory Menu

The Directory menu is activated by selecting the Set Directory button in the Files Main menu, by selecting Return in the Directories Secondary menu, or by entering the command `files('files_dir')`.

Button	*Description*
Change	Change to a new directory. First, mark a directory in the files display (directories have a "`/`" following their names) and then click on this button. If you have selected a directory, that becomes the new current directory. If you have not selected any entries, a prompt appears requesting the name of the new current directory.
Default	Set current directory to the value of parameter `defaultdir`. Initial value is your home or login directory.
Set Default	If you click this button and haven't marked any entries, the current directory becomes the new value of parameter `defaultdir`. Otherwise, if you have marked a directory and then clicked on this button, the directory you marked becomes the new `defaultdir`. In both cases, the new value of `defaultdir` is displayed. An error is reported otherwise.
Parent	Set the current directory to the parent of the current directory.
Home	Set the current directory to the home or login directory.
Nmr	Set the current directory to your VNMR user directory, which has your VNMR experiments, `maclib`, `menulib`, etc.
More	Display the Directory Secondary menu (below).
Return	Display the Files Main menu (page 87).

Directory Secondary Menu

The Directory Secondary menu is activated by selecting the More button in the Directory menu or by entering `files('files_dir_2')`.

Button	*Description*
VNMR	Set the current directory to be the VNMR system directory.
Create New	Show prompt "`New directory (enter name and <return>)?`", then create directory with the name entered and set the current directory to be this new directory. If done successfully, the `files` display will have no entries because the new current directory just created is empty.
Return	Display the Directory menu (above).

Files Information Menu

The Files Information menu is activated by selecting the Files Info button in the Files Main menu or by entering `files('files_info')`.

Button	*Description*
By Size	Sorts the entries in the current directory by size. Largest files are listed last. For subdirectories, the size of the entries in the subdirectory is included in figuring the size of the entry. The resulting sorted list is displayed in the VNMR text window.
By Date	Sorts the entries in the current directory by the date each was last modified, with entry most recently modified listed last. Resulting sorted list is displayed in the VNMR text window.
Return	Display the Files Main menu (page 87).

Files Tape Menu

The Files Tape menu handles UNIX tapes only (used on UNITY*INOVA*, UNITY*plus*, *MERCURY-VX*, *MERCURY*, *GEMINI 2000*, UNITY, and VXR-S systems). The Files Tape menu is activated by selecting the Tape button in the Files Main menu or by entering `files('files_tape')`. The `tape` parameter defines the device the files program accesses when it is instructed to read or write to a tape.

Button	*Description*
Directory	Displays the contents of the streaming tape currently loaded in the tape drive. Since UNIX `tar` tapes do not have a directory per se, the entire tape must be read in order to produce this listing, so the operation may be time-consuming.
Sizes	Reports the size of each entry in the current directory. To report the size of selected entries only, mark one or more entries in the `files` display first and then click on this button. The size of the entries you marked is reported in the VNMR text window. The size of each entry in a subdirectory is included in figuring the size of the subdirectory.
Write	Write the entire contents of the current directory to tape. To write selected entries only to tape, mark one more entries in the `files` display first and then click on this button. Only those entries you marked are written to the tape.
Read All	Load contents of the streaming tape into the current directory.
Return	Display the Files Main menu (page 87).

Files Data Menu

The Files Data menu is activated by selecting Data in the Files Main menu or by entering `files('files_data')`.

Button	*Description*
Load	First mark one file in the `files` display and then click on this button. If you have selected an entry that has Varian NMR data, including data from a Gemini, VXR, or XL system, that parameter set and data is loaded into the current experiment. If it is a parameter set only, the parameters are loaded.
Save FID	Show prompt "`File name (enter name and <return>)?`" and save data in current experiment there.
Show Shims	Show the contents of the system `shim` directory (the `shim` directory in the VNMR system directory) and the user `shim` directory (the `shim` directory in your VNMR user directory).
Load Shims	First mark one file in the `files` display and then click on this button. If you have selected an entry that is an NMR data set, the program loads the shims stored with that NMR data. Otherwise, the program assumes the entry is a shim data set and attempts to load the shims from that entry.
Save Shims	Show prompt "`File name (enter name and <return>)?`" and save shims in current experiment there.
More	Display the Files Data Secondary menu (below).
Return	Display the Files Main menu (page 87).

Files Data Secondary Menu

The Files Data Secondary menu is activated by selecting More in the Files Data menu or by entering `files('files_data2').`

Button	*Description*
Load Params	Start by marking one file in the `files` display, and then click on this button. If you have selected an entry that has NMR data, the parameters from that data are loaded into the current experiment.
Save Params	Show prompt "`File name (enter name and <return>)?`" and save the parameters from the current experiment there.
Return	Display the Files Main menu (page 87).

Files Secondary Menu

The Files Secondary menu is activated by selecting More in the Files Main menu or by entering `files('files_main2')`. To mark a file, place the mouse cursor over the file name and click the left mouse button. The file name will appear in reverse video when marked. To deselect a file name, click on it again.

Button	*Description*
Display	Start by marking one or more files in the `files` display, and then click on this button to display the files you marked. This action is appropriate for text files only.

Button	*Description*
Edit	Start by marking one or more files in the `files` display, and then click on this button to edit the files you marked. This action is appropriate for text files only.
Copy	Start by marking one file in the `files` display, and then click on this button to make a copy of the file you marked. You are asked for the name of new file.
Rename	Start by marking one file in the `files` display, and then click on this button to rename the file you marked. You are asked for the new name of new file.
Return	Display the Files Main menu (page 87).

4.13 Secondary Main Menu

Selecting More in the Main menu activates the Secondary Main menu, a series of additional choices that do not fall into one of the other main categories. Of these, the most important button will probably be Exit VNMR, which you should routinely use when you are ready to terminate your session at your spectrometer or data station. You can also activate the Secondary Main menu by entering `menu('main2')`.

Button	*Description*
Write Pulse Sequence	Display the Pulse Sequence Entry Main menu (below) to initiate menu-driven pulse sequence generation.
Configure	Display the Configuration menu (page 92) to modify the system configuration, such as selecting a plotter.
UNIX	Open a temporary UNIX shell. This shell becomes the active process, superseding the VNMR software. When finished, use the right mouse button to select Quit, or press Control-d to terminate the process and display the Main menu (page 66).
Exit VNMR	Exit the VNMR program, returning to a UNIX shell. All data in your temporary NMR files are saved.
Return	Display the Main menu (page 66).

Pulse Sequence Entry Main Menu

The Pulse Sequence Entry Main menu is typically entered by selecting Write Pulse Sequence in the Secondary Main menu or by entering `menu('psg_main')`. This menu is the first of seven menus to assist you in generating pulse sequences. For detailed information about the menus and on menu-driven pulse sequence programming, refer to Chapter 2, “Pulse Sequence Programming,” in the manual *VNMR User Programming*.

Configuration Menu

The Configuration menu is activated by selecting the Configure button in the Secondary Main menu or by entering `menu('configure')`.

Button	*Description*
Show Output Devices	Show all printer and plotter output devices that have been defined as active on this system.
Select Plotter	Select the next plotter on the list in `/vnmr/devicenames`.
Select Printer	Select the next printer on the list in `/vnmr/devicenames`.
Hardware	Enter the `config` program (the NMR system administrator `vnmr1` must use `config` at least once to set up the proper system hardware configuration).
Return	Display the Main menu (page 66).

Chapter 5. Using the Command Mode

Sections in this chapter:

- 5.1 “Commands” this page
- 5.2 “Parameters” page 94
- 5.3 “Command Line Editing and Reentry” page 96
- 5.4 “Macro Automation” page 98

Commands, macros, and parameters can be entered by typing them in the VNMR input window, by clicking on certain buttons in the VNMR menu system, or by setting values interactively in the *GLIDE* window. When commands, macro, and parameters are entered in the input window, it is called the *command mode*.

A *command* is a request to have an action performed. A *macro* is also a request to have an action performed, but the macro action can be customized by users because the source code is readily available (making changes to commands can only be done if the user purchases the optional VNMR Source Code Kit). A *parameter* shapes the action that commands take.

The command mode allows access to all commands, macros, and parameters, while the other two modes, menu system and *GLIDE*, allow access to *some* commands, macros, and parameters only. Thus, the emphasis of this section, and of the manual as a whole, is on providing information about interacting with the system in the command mode. Keep in mind, however, that use of the menu system and *GLIDE* provide a convenient shortcut to most routine operations and, in typical use, you may work for minutes or even hours without touching the keyboard.

For detailed descriptions of all commands, system macros, and parameters, refer to the *VNMR Command and Parameter Reference*.

5.1 Commands

Command names contain a variable number of alphanumeric characters (e.g., `go`, `jexp1`, and `dcon`). Commands can be divided into four types, as follows:

- *Commands with no arguments* – The command `eject`, for example, stands by itself.
- *Commands requiring one or more arguments* – The command `svf` (save an FID file on disk), for example, requires the input of the name of the FID file. The needed argument is enclosed in parentheses using the syntax `svf(file)`. Because a file name is a text string, the file name is required to be enclosed in single quote marks when entered: `svf('/export/home/vnmr1/mydatafile')`. Numbers and variables (such as parameters) do not require the single quotes. If two or more arguments are required, each argument is separated by a comma.
- *Commands with optional arguments* – A good example here is `ds<(index)>` (the angled brackets identify optional arguments). To display a 1D spectrum, the command

is `ds`. However, if a series of spectra have been acquired, the number of the spectrum to be displayed can be specified, as in the command `ds(3)`.

- *Interactive commands* – An interactive command obtains information by asking the operator questions. For example, when the command `dot1` is entered, the system displays a series of prompts that guide the operator in setting up a T_1 experiment.

Command Entry

Commands are entered by typing the name of the command, typing the command arguments (if appropriate) in parentheses, and then pressing the Return key. There should never be a space between the command name and the left parenthesis (e.g., `ds (3)` is incorrect). More than one command can be entered at the same time for sequential execution by separating each command with a space (e.g., type `ds(3) pl pa` and press Return). Commands and parameters can also be interspersed on input (e.g., `nt=16 at=2.0 go`).

Command Arguments

Arguments for commands come in two types—numeric and string:

- *Numeric arguments* can be integer or real (although integer parameters are stored as real), and can be entered with or without a decimal point (e.g., `16`, `16.0`, `16.5`).
- *Strings* are distinguished by being enclosed in single quote marks (`'...'`), such as `'SAMPLE 12'` or `'3456'`.

Any character can appear between the single quotation marks, but a few special characters, such as a single quotation mark, must be proceeded with a backslash (\) if the character is to be enclosed within a text string, for example,

```
'You can\'t enter a single quote without special care'.
```

To insert a backslash character itself in a string, it must be used twice (e.g., *A\B* is written `'A\\B'`).

As do numeric arguments, the string becomes an argument by appearing inside parentheses. For example, by using the command `text`, the operator can store alphanumeric text in a file that accompanies the current experiment. Thus, to record a sample number and date, the operator can enter `text('SAMPLE 307-3May')`.

Some text arguments are free-form, as in the `text` command just described. In other cases, however, certain specific values of a text string are required. For example, the command to plot a contour plot is `pcon`. If you want to plot only the positive contours of a phase-sensitive experiment, then you enter `pcon('pos')`. The text string `'pos'` and others like it are referred to as *keywords*. A keyword must be entered exactly as shown in VNMR manuals and on-line.

5.2 Parameters

Parameter names have a variable number of alphanumeric characters (e.g., `nt`, `temp`, `axis`). There are only two types of parameters: numeric and string. Numeric parameters are numbers, while string parameters are a collection of one or more letters.

Numeric parameters that are typically integers, such as `nt` (number of transients), can be entered with or without a decimal point (e.g., `16` or `16.0`). Scientific notation is also acceptable for input (e.g., `1e3` for 1×10^3 or `2.5e-4` for 2.5×10^{-4}).

Suffixes p, d, and k have been given the following meaning when inputting numeric parameters:

- The p suffix translates the input to ppm units. For example, entering sw=10p is equivalent to entering sw=(10*reffrq).
- The d suffix translates the input to ppm units relative to the decoupler frequency. For example, entering sw1=10d is equivalent to entering sw1=(10*reffrq).
- The k suffix translates the input to thousands. For example, fn=16k (setting the Fourier number parameter to 16k) is equivalent to fn=(16*1000). Note, however, that fn=16k is internally calculated to a power of 2; therefore, fn=16k actually sets the Fourier number to 2^{16} or 16384.

These definitions of p, d, and k are made in the bootup macro with the command unit. Additional suffixes can be defined and p, d, and k can be redefined with the unit command.

Mathematical expressions can contain numbers with these suffixes, so you can enter, for example, sw=10p+tof-2k.

A string parameter takes a variable-length alphanumeric string as a value. The strings are always enclosed within single quotation marks ('...'). For example, the value of dmm (decoupler modulation mode) might be 'c', while the value of dm (decoupler mode) might be 'nyy'. Many alphabetic parameters have values of 'y' for yes and 'n' for no.

By setting a parameter to the 'n' value, certain numeric parameters are capable of being "turned off." The parameter temp for probe temperature is an example. To select a temperature of 60°C, type temp=60; to turn off the temperature regulation, type temp='n'. A parameter that is deactivated by setting its value to 'n' can be reset to its last numeric value by entering a value of 'y'. For example, if the current value of line broadening is 1.5 (i.e., lb=1.5), you can deactivate line broadening with lb='n'. A subsequent lb='y' will restore the value of lb to 1.5.

Parameter Entry

All parameters are entered the same way—type the name of the parameter, an equals sign, the value, and then press the Return key. For example, to set the parameter sw to 1000, type sw=1000 and press Return. Or to turn off temperature regulation, type temp='n' and press Return. To input more than one parameter at the same time, separate each parameter entry with a space and press Return after the last entry; for example, type nt=16 dm='yyy' temp=40 and press Return. (To avoid repetition in this manual, pressing the Return key after each entry should be assumed and will not be mentioned except in special cases.)

Parameters can be arrayed by entering a series of values separated by commas. Both numeric parameters and string parameters can be arrayed in this fashion. For example, entering nt=1,1,1,1 or dm='nnn','nny' makes nt or dm an arrayed parameter. For easy entry of linearly spaced array values, you should use the array macro.

To change a specific element of an arrayed parameter, provide the array index in square brackets ([...]) to access the element (e.g., nt[3]=2 sets the third value of the nt array to 2). Multiple elements of an array can also be altered or added by entering a series of values. Again using the nt example, nt[5]=4,4,4,4 adds elements 5, 6, 7, and 8 to the nt array and sets the value of each of these elements to 4.

Parameter Display

To display the current value of any parameter, type the name of the parameter, followed by a question mark "?" (pressing the Return key is assumed). For example, to find the value of `sw`, type `sw?` and the monitor displays the value of `sw`. Unlike parameter entry, only one parameter value can be requested at a time.

If the parameter to be displayed is an arrayed parameter, the number and type of array elements are displayed. For example, if `nt` is arrayed, entering `nt?` might display the message "`nt=array of 8 reals`."

To display an individual element of an array, provide the index in square brackets (e.g., `nt[3]?` might display "`nt[3] = 2`").

Certain parameters can be "turned off" by setting the parameter to `'n'`. The display of a parameter that is turned off is the phrase "Not Used" followed by the actual value in parentheses. For example, if `lb` is set to 1.5 and then set to `'n'`, entering `lb?` will display `lb= Not Used (1.5)`.

Parameter Value Limitations

Some parameters have restricted value ranges. The parameter `nt` (number of transients) cannot be negative, for example. Attempting to enter an illegal value results in the system assigning the parameter a minimum or maximum value. An error message is also displayed explaining the actual value assigned to the parameter.

Certain numeric parameters, `nt` is an example again, are limited to integers, and a non-integer number entered is rounded to the nearest integer.

Some string parameters can only be set to enumerated string values. Attempting to enter a value that is not one of these values produces an error message, and the parameter is unchanged. Similarly, some flag parameters can only be set to enumerated characters. Attempting to enter a character string containing a character that is not one of the enumerated characters of a flag parameter produces an error message, and the parameter is unchanged.

Entering parameters may not have an immediate effect. For instance, if `temp=60` is entered, no temperature is regulated until an acquisition is started with the `go` command or until the hardware setup command `su` is executed.

Parameter Entry Limitations

Some parameters, such as `ct` (number of completed transients), cannot be entered from the keyboard. Attempting to enter such a parameter in the normal way produces the error message that the assignment is not allowed.

5.3 Command Line Editing and Reentry

You can reenter a command or series of commands that you previously typed. Editing the previous or current commands is accomplished with the arrow keys, special keys, and key combinations. For details, move the mouse to the VNMR input window, hold down the Control key, and press the right mouse button to open an instruction menu window.

Perhaps you entered the command `cat('/vnmr/psglib/noesy.c')` to display a particular pulse sequence. You thought you saw what you wanted, but a few minutes later you need to enter the same command again. Rather than retype that long file name, you can

press the up-arrow key (marked ▲) or enter Control-P (hold down the Control key and then press the P key) to recall your command.

Each time you press the up-arrow key or enter Control-P, the previous line is recalled (think of the "P" in Control-P as standing for "previous"). Depending upon how much you have been typing, you may be able to go backwards in time several minutes or even several hours. If you go back too far, the down-arrow key (marked ▼) or Control-N moves to the next line. For example, pressing Control-P Control-P Control-N moves back two lines and then down one line.

Once you have recalled a previous line, you can edit the line with these keys:

Left-arrow	Move left one character (alternate: Control-H).
Right-arrow	Move right one character (alternate: Control-L).
Delete or Backspace	Delete a character.
Control-U	Delete the entire line.

Insertion is accomplished by typing the desired character. When the line is correct, press Return as usual to enter the line. The cursor does not have to be moved to the end of the line before you press Return.

Command line editing is also active on the current line, that is, before you have pressed Return for the first time. If you notice an error in a line you are typing, press left arrow, or Control-H to return to the error, press Delete to erase the characters you do not want, type in the correct characters, and then press Return.

Press the left mouse button and drag the cursor to highlight the words or characters to be cut or copied. Press the Cut key to remove the highlighted words or characters. Press the Paste key or mouse button 2 to paste the selected or cut words/characters.

Table 4 summarizes the key actions described in this section. Note that these key actions can be changed with the UNIX `stty` command.

Table 4. Special Keys for VNMR Line Editing

Key	
Left-arrow, Control-H	Move left one character without deleting
Control-Left-arrow	Move cursor left to previous word
Control-Backspace	Deletes all characters before cursor
Right-arrow, Control-L	Move right one character
Control-Delete	Delete all characters following cursor
▲, Control-P	Recall command previously entered
▼, Control-N	Move to next line
Delete, Backspace	Delete one character
Control-mouse button 1	Move cursor to position of pointer
Control-U	Delete entire line
Return	Terminate end of one line of input
End	Moves cursor to end of line
Cut	Delete all selected characters
Paste, mouse button 2	Paste characters that are selected or cut
Undo	Undo previous paste of delete

5.4 Macro Automation

Many experiments can be automated by using macros supplied with the system software, by modifying system macros, or by running user-written macros. Many system macros are available. The majority were developed to run as a part of *GLIDE* interface or to automate systems with sample changers, but they can be used directly by the user or modified as needed.

The following tables in this section list automation macros according to type:

- Table 5 lists automated acquisition macros.
- Table 6 lists automated calibration macros.
- Table 7 lists automated plotting macros.
- Table 8 lists automated processing macros.

For further information about these macros, refer to the entry for the macro in the *VNMR Command and Parameter Reference* or examine the source code for the macro in the `maclib` directory.

Table 5. Automated Acquisition Macros

Macros	
`autolist*`	Set up and start chained acquisition
`c13<(solvent)>`	Automated carbon acquisition
`capt<(solvent)>`	Automated carbon and APT acquisition
`cdept<(solvent)>`	Automated carbon and DEPT acquisition
`f19<(solvent)>`	Automated fluorine acquisition
`getdim:dimensions`	Return dimensionality of experiment
`h1<(solvent)>`	Automated proton acquisition
`hc<(solvent)>`	Automated proton and carbon acquisition
`hcapt<(solvent)>`	Automated proton, carbon, and APT acquisition
`hccorr<(solvent)>`	Automated proton, carbon, and HETCOR acquisition
`hcdept<(solvent)>`	Automated proton, carbon, and DEPT acquisition
`hcosy<(solvent)>`	Automated proton and COSY acquisition
`p31<(solvent)>`	Automated phosphorus acquisition
`* autolist(<option,>experiment1<,experiment2<,experiment3,...>)`	

Table 6. Automated Calibration Macros

Macros	
`AC1S-AC11S`	Autocalibration macros
`ACbackup`	Print copy of probe file after autocalibration
`ACreport`	Make backup of current problem file

Table 7. Automated Plotting Macros

Macros	
`pacosy`	Plot automatic COSY analysis
`plapt<(13Cexp_number)>`	Plot APT-style spectra automatically
`plarray`	Plot arrayed 1D spectra
`plc<(pltmod)>`	Plot a carbon spectrum
`plcosy*`	Plot COSY- and NOESY-type spectra automatically
`plh<(pltmod)>`	Plot proton spectrum
`plhet2dj*`	Plot heteronuclear J-resolved 2D spectra automatically
`plhom2dj*`	Plot homonuclear J-resolved 2D spectra automatically
`plhxcor*`	Plot X,H-correlation 2D spectrum
`plot`	Plot spectra automatically
`plot1d`	Plot simple (non-arrayed) 1D spectra
`plp<(pltmod)>`	Plot phosphorus spectrum
`* plcosy(<'pos'|'neg'><,><levels<,spacing<,exp1D>>>)`	
`plhet2dj(<'pos'|'neg'><,><levels<,spacing<,exp1D>>>)`	
`plhom2dj(<'pos'|'neg'><,><levels<,spacing<,exp1D>>>)`	
`plhxcor(<'pos'|'neg'><,><levels<,spacing<,exp1D_H<,exp1D_X>>>>)`	
Parameter	
`parstyle` {string}	Parameter style to plot

Table 8. Automated Processing Macros

Macros	
`autostack`	Automatic stacking for processing and plotting arrays
`c13p`	Processing of 1D carbon spectra
`cleanexp<(file1<,file2<,...>>)>`	Remove old files and directories from an experiment
`cptmp<(file)>`	Copy experiment data into experiment subfile
`f19p`	Process 1D fluorine spectra
`get1d<(experiment)>`	Select a 1D experiment for processing
`get2d<(experiment)>`	Select a 2D experiment for processing
`h1p`	Process 1D proton spectra
`hregions`	Select integral regions in proton spectrum
`integrate`	Automatically integrate 1D spectrum
`isadj<(height<,neg_height>)>`	Automatic integral scale adjustment
`isadj2<(height<,neg_height>)>:sf`	Automatic integral scale adjustment by powers of two
`p31p`	Process 1D phosphorus spectra
`proc1d`	Process simple (non-arrayed) 1D spectra
`proc2d`	Process 2D spectra
`procarray`	Process arrayed 1D spectra
`process`	Generic automatic processing
`procplot`	Automatically process FIDs
`rttmp(file)`	Retrieve experiment data from experiment subfile
`stack(mode)`	Fix stacking mode for processing and plotting spectra
`svtmp<(file)>`	Move experiment data into experiment subfile
Parameters	
`pkpick` {string}	Peak pick
`stackmode*`	Stacking control for processing arrayed 1D spectra
* `stackmode` {'horizontal','vertical','diagonal'}	

Chapter 6. Preparing for an Experiment

Sections in this chapter:

- 6.1 “Preparing the Sample” this page
- 6.2 “Ejecting and Inserting the Sample” page 103
- 6.3 “Retrieving Parameter Sets” page 106
- 6.4 “Removing and Inserting the Probe” page 112
- 6.6 “Tuning the Probe” page 113
- 6.7 “Spinning the Sample” page 127
- 6.8 “Optimizing Lock” page 130
- 6.9 “Adjusting Shims” page 135
- 6.10 “Using the Acquisition Window” page 148
- 6.11 “Shimming Using the Ultra•nmr Shim System” page 164
- 6.12 “Gradient Autoshimming” page 168

These sections are in the same order as typically performed by most users.

6.1 Preparing the Sample

Reliable and fast accumulation of data from multiple samples depends greatly on the way samples are prepared and positioned in the turbines, and the autoshimming methods and lock power used. Variations in bulk magnetic susceptibility at air-to-glass, glass-to-solvent, and solvent-to-air contact points can contribute a dominant portion of the variation of field homogeneity from sample to sample, whether in an automation run or in manual operation. The time spent shimming, or even the need to shim is largely dependent on the care in controlling the effects of these contact points.

Solvent Selection

Samples can be run as neat liquids or in solutions. In most cases, you will probably be running compounds in solution. The solution should be chosen to be inert (does not react with the sample) and available in deuterated form. The instrument can be run unlocked, that is, without locking onto the deuterium of a deuterated solvent, but resolution is better with a deuterium lock, especially for lengthy accumulations. Probably the most commonly used solvents are deuterated acetone, chloroform, methylene chloride, and DMSO.

Sample Height

Experimentation and calculation show that the liquid column length must be at least three times the length of the observe coil to minimize end effects. This suggests a column length

of close to 5 cm for a standard broadband or switchable probe, and about 4 cm for a $^{1}H/^{19}F$ probe. Solvent volumes of 0.6 ml in a 5-mm tube and 3.1 ml in a 10-mm tube are adequate for removing the end effects.

Reduction of sample volume to attain higher concentration usually fails because the increased signal is found around the base of the NMR resonance, not within the narrow portion of the signal. In fact, a well-shimmed 0.4 ml sample will be lower in sensitivity than the same solution diluted to 0.6 ml and also shimmed well. The questionable gain in sensitivity is further degraded by the longer time it will take to shim the system. Small variations of sample height that would be insignificant in a 0.6 to 0.8 ml sample can be dominant when the sample is only 0.4 ml in volume.

For best results and minimum shimming time, samples should be prepared to be the same height as much as possible. Above 0.7 ml there is little sensitivity to sample length as long as the bottom of the tube is positioned properly. You should make every sample up to the same height and obtain your shim values using samples of that height.

For Wilmad 528 or 535 tubes with no restricting plugs, typical samples with volumes listed in Table 9 should be placed at the depths shown in the table, where depth is the distance in mm from the bottom of the green spinner turbine to the bottom of the sample tube.

Table 9. Sample Tube Depths

Volume	*Length*	*Depth (Range)*
700 µL	50 mm	68 mm (65–69 mm)
600 µL	42 mm	65 mm (63–67 mm)
500 µL	36 mm	62 mm (60–64 mm)
400 µL	28 mm	59 mm (58–62 mm)

Sample Position

Use the depth indicator provided to set the sample position to a repeatable position. Figure 21 shows the depth indicators on the spectrometer for 10-mm and 5-mm sample tubes. The larger spinner is available in both 10-mm and 5-mm versions.

To Position a Sample Using the Depth Indicator

The procedure here is for the 5-mm tube using the larger spinner. Other tube sizes and spinners are done similarly.

- Place the bottom of the flange along the line indicated in the figure, and lower the sample until the sample tube bottom equals the “Maximum Sample Depth” line for the smaller 5-mm sample tube.

  The length from the bottom of the flange to the bottom of the sample tube should not exceed 124 mm. If you need to use less than 0.7 ml of solvent for any reason, you can center the liquid volume in the cross-hatched area. This centers the sample in the receiver coil, indicated by the center line symbol.

To Position a Sample Using the Sample Tray

Alternatively, if using the sample changer, the sample tray itself can be used to set an appropriate depth for the bottom of the NMR tube. This procedure, if followed for all samples placed in the tray, results in a very reproducible sample position and, once shim settings have been determined for this length of sample, there should be very little shimming necessary when changing samples, even with a solvent change.

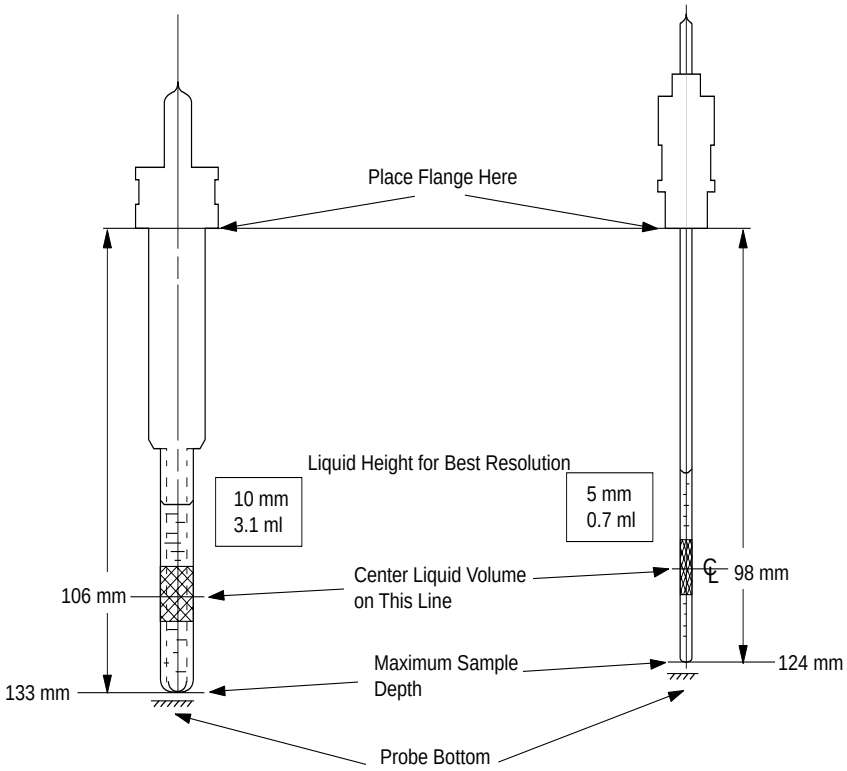


Figure 21. Sample Depth Indicator

- Insert the NMR tube into the turbine and gently push the tube down through the turbine while holding the turbine/tube combination in the other hand *within location zero*. When the tube touches the bottom, stop pushing down.

  The sample is now properly positioned. If too much pressure is applied the bottom of the tray may flex and when released the tube make rock slightly within the hole. If so, back out the tube a fraction of a millimeter to seat the turbine firmly without rocking. Location zero is fitted with a more rigid bottom and better resists flexing.

Sample Tubes

Finally, it is helpful to buy the best quality NMR sample tubes and to clean the outside of each tube with a solvent such as isopropyl alcohol, followed by a careful wiping with a wiper tissue before placing the tube in the probe.

6.2 Ejecting and Inserting the Sample

On *MERCURY-VX*, *MERCURY*, *GEMINI 2000*, UNITY*INOVA*, UNITY*plus*, UNITY, and VXR-S spectrometers with automatic insert/eject, the spectrometer is equipped with hardware and software to provide computer control of sample ejection, insertion, spinning, locking, and shimming. This section covers computer-controlled sample ejection and insertion. Table 10 lists the commands and parameters related to sample changing.

Manual control of ejection and insertion is also provided on each of these systems to enable you to withdraw samples if necessary, but it is strongly recommended that you rely on computer control for maximum reproducibility and safety. On *MERCURY* and *GEMINI*

Table 10. Sample Changing Commands and Parameters

Commands	
`acqi*`	Interactive acquisition display
`change`	Submit change sample experiment to acquisition
`e, eject`	Eject sample
`i, insert`	Insert sample
`sample`	Submit change sample, autoshim experiment.
`* acqi<('par'|'disconnect'|'exit'|'standby')><:ret>`	
Parameters	
`loc {0, 1 to traymax}`	Location of sample in tray
`traymax {0, 9, 50, 100}`	Sample changer tray size

2000 spectrometers, manual control is the only way to withdraw samples unless the optional spinner control board is installed in the system.

Solids probes do not support sample insertion and ejection.

To Eject a Sample, Without a Sample Changer

You should always eject first (even if no sample is in the magnet) to start airflow to carry the sample. The ejection air is turned on and, under computer control, the sample, if present, rises back to the top of the upper barrel. You can now remove the sample and replace it with another sample.

Using the Input Window

Applies to all systems if the optional spin control hardware is installed.

- Enter **`e`** in the input window.

Using GLIDE

Applies to all systems if the optional spin control hardware is installed.

1. If the *GLIDE* interactive window is not open, open it entering **`glide`** in the input window or by clicking on the **GLIDE** button in the Main Menu.
2. Click on **Experiment & Solvent** > **Eject** > **Close**.

Using the Acquisition Window

Applies to systems configured for acquisition if the optional spin control hardware is installed.

1. If the Acquisition window is not open, enter **`acqi`** in the input window, then click on the **Connect** button in the window when it appears.
2. In the SAMPLE menu, click on the **eject** button.

Manual Ejection

Applies to systems *without* spin control hardware. *It is used only in emergencies on other systems*.

- Press the black button on the top of the left leg of the magnet.

To Insert a Sample, Without a Sample Changer

When inserting a sample, the sample tube gradually lowers down the upper barrel under computer control. After a five-second delay, the bearing air is turned off momentarily, allowing the turbine to seat properly.

The two-stage sample insertion operation is provided for safety reasons, particularly when working with the 5 mm upper barrel, which uses smaller turbines. Because the tube itself is used as the bearing surface in this barrel, the tube must drop down the barrel slowly enough to avoid breaking when contact is made with the conical guide. The second stage drop then permits the tube to slide into the bearing cylinder. Operation using the larger upper barrel, which can hold 5-, 10- and 16-mm tubes, is less susceptible to these problems because the turbine makes initial contact and alignment before the sample tube encounters any close tolerance.

Using the Input Window

Applies to all systems if the optional spin control hardware is installed.

1. Perform a sample ejection (even if no sample is in the magnet) to start airflow to carry the sample.
2. Insert the sample by placing it in the top of the upper barrel.
3. Enter **`i`** in the VNMR input window.

Using GLIDE

Applies to all systems if the optional spin control hardware is installed.

1. If the *GLIDE* interactive window is not open, open it entering **`glide`** in the input window or by clicking on the **GLIDE** button in the Main Menu.
2. Click on **Experiment & Solvent** > **Eject**.
3. Insert the sample.
4. Click on **Insert** > **Close**.

Using the Acquisition Window

Applies to all systems configured for acquisition if the optional spin control hardware is installed.

1. Perform a sample ejection (even if no sample is in the magnet) to start airflow to carry the sample.
2. Insert the sample by placing it in the top of the upper barrel.
3. If the Acquisition window is not open, enter **`acqi`** in the input window, then click on the **Connect** button in the window when it appears.
4. In the SAMPLE menu, click on **insert**.

Manual Ejection

Applies to systems without spin control hardware. Used only in emergencies on other systems.

1. Press the black button on the top of the left leg of the magnet.
2. Insert the sample by placing it in the top of the upper barrel to start airflow.

3. *Slowly* release the black button to slowly drop the sample. When the button is completely released, close off the top of the upper barrel with your hand for a second to properly seat the sample.

To Change a Sample, With a Sample Changer

Only if the sample changer is disabled by setting `traymax=0` or `loc=0` (perhaps during daytime walk-up operation) should you work with samples as described above.

- If a sample changer is in use and a sample is ejected using *GLIDE*, the `e` macro, or the Acquisition window, the changer no longer has any way of knowing which sample is in the magnet. When the next sample is loaded by the sample changer, it will place the current sample in location zero.
- If a sample is changed manually (using the button on the magnet leg), the sample changer will still think the previous sample is present and will return the sample in the magnet to that location when it is activated.

The following procedures change only one sample at a time on a sample changer. Refer to the chapter on sample changers in *User Guide: Liquids NMR* for automated changing of multiple samples.

Using the Input Window

1. Place the samples you want to insert in the sample tray.
2. Enter **`loc=`*`n`*` change`** in the input window, where *n* is the location on the tray where you want the sample to be taken (e.g., to remove the sample in location 5, enter `loc=5 change`).

   The `change` macro removes the sample currently in the probe and places it in the last position used by the changer, or if none had been previously specified, the sample is placed in the location 0. The sample changer arm then picks up the sample in the location specified by `loc` and inserts it into the probe.

   The `sample` macro performs the combined operations `change`, `spin`, `lock`, and `shim`, convenient for setting up a new sample on a system with a sample changer.

Using GLIDE

1. If the *GLIDE* interactive window is not open, open it entering **`glide`** in the input window or by clicking on the **GLIDE** button in the Main Menu.
2. Click on **Experiment & Solvent**.
3. In the space after Location, enter the location where you want the sample placed.
4. Click on **Close**.

   The system recalls parameters and performs the actions described for the `change` command above.

6.3 Retrieving Parameter Sets

At any given time, you are joined to an experiment with a particular set of parameters. These parameters remain active until they are changed. Thus, to repeat an experiment you have just performed, no parameter setup is necessary—just start the acquisition.

If you just need to change one or two parameters from the previous experiment in order to set up the next experiment, that can be done by entering those parameters in the input window (e.g., `pw=6 nt=16`). Refer to “Setting Frequency-Related Parameters” on page 183 and “Setting Pulse-Sequence-Related Parameters” on page 185 for a description of these parameters.

If many parameters have to be changed, you could enter the parameters one by one, but a much better method would be to recall a parameter set that describes exactly, or at least approximately, the experiment you wish to do. That is the topic of this section—how to set up an experiment using saved parameter sets, including the standard parameters sets shipped with VNMR. Table 11 summarizes the commands and parameters used in this section.

Table 11. Retrieving Parameter Sets Commands and Parameters

Commands	
`addpar*`	Add selected parameters to the current experiment
`cd<(directory)>`	Change working directory
`dg<(template)>`	Display group of acquisition/processing parameters
`dg1`	Display group of display parameters
`dg2`	Display group of 3rd/4th rf channel/3D parameters
`dglp`	Display group of linear prediction parameters
`dgs`	Display group of shim and automation parameters
`fixpar`	Correct parameter characteristics in experiment
`fixpar3rf`	Create parameters for third rf channel
`fixpar4rf`	Create parameters for fourth rf channel
`fixpar5rf`	Create parameters for fifth rf channel
`lf<(directory)>`	List files in the current directory
`paramedit(parameter<,tree>)`	Edit parameter and attributes with user-set editor
`paramvi(parameter<,tree>)`	Edit a parameter and attributes using vi editor
`rtp<(file)>`	Retrieve parameters
`setup<(nucleus<,solvent>)>`	Set up parameters for basic experiments
`userfixpar`	Macro called by fixpar
`* addpar<('2d'|'3d'|'3rf'|'4d'|'downsamp'|'fid'|'image'|ll2d'|'lp'<,dim>|'oversamp'|'ss')>`	
Parameters	
`dg` {string}	Control dg parameter group display
`dg1` {string}	Control dg1 parameter group display
`dg2` {string}	Control dg2 parameter display
`dgs` {string}	Control dgs parameter group display
`file` {string}	File name of parameter set

Location of Parameter Sets

Parameter sets are organized into a number of files and placed in directories:

- Directory `/vnmr/stdpar` contains standard parameter sets for different nuclei. For example, `/vnmr/stdpar/H1.par` contains parameters for running routine ^{1}H spectra and `/vnmr/stdpar/C13.par` contains parameters for ^{13}C spectra.
- Directory `/vnmr/parlib` contains parameters sets for particular experiments, such as `/vnmr/parlib/dept.par` and `/vnmr/parlib/hmqc.par`.
- Directory `/vnmr/tests` contains parameter sets for the standard system tests, such as `/vnmr/tests/H1lsph` for lineshape and `/vnmr/tests/C13sn` for signal-to-noise.

- Similarly, on your system, directories `stdpar` and `parlib` are standard for every user in `vnmrsys`. These directories are empty at first but grow with parameter sets from experiments that you and other users on your system have saved. Normally, you save parameter sets into your home directory. (Chapter 10, “Storing, Retrieving, and Moving Data,” describes how to save user data.)

To List Parameter Sets

You can list parameter sets using the menu system or by entering the `lf` command.

Using the Menu System

1. Click on **Main Menu** > **File**

   The File menu appears with the following buttons:

   In the graphics windows is a list of files and directories (the directory entries have a slash at the end, for example, `stdpar/`) for the current directory.

2. To examine the `stdpar` or `tests` standard system parameter sets, you need to be in `/vnmr/stdpar` or `/vnmr/tests`. To examine local parameter sets, you need to be in the appropriate user directory. In either case, you are probably not in the directory you want. To change directories, click on **Set Directory**.

   The Directory menu appears with the following buttons:

3. Repeatedly click on **Parent** until the entry for the top-level directory you want appears (e.g., `vnmr/`).

   If you have saved parameter sets in your home directory, click on the Home button to immediately display the files there.

4. Move down to the subdirectory you want (e.g., `stdpar/`) by clicking on the entry for the next subdirectory in the path with the left mouse button so that the entry reverses (instead of dark type with a white background, the background is dark and the type is white) and then clicking on **Change**.

   Repeat this step until you can view the entries for the directory you want. For example, for the standard parameter set directory `/vnmr/stdpar`, the entries shown are typically for following directories:

   ```
   C13.par/ F19.par/ H1.par/ H2.par/ N15.par/ P31.par/
   ```

Using the Input Window

- Enter the command **`lf<(`*`directory`*`)>`** where *`directory`* is the name of the directory containing the parameter sets (e.g., `lf('/vnmr/stdpar')` or `lf('/vnmr/tests')`).

  To list parameters sets (if any exist) in your home directory, enter `cd`, then `lf`. The command `cd` with no argument changes to your home directory by default.

To Recall Any Parameter Set

You can retrieve an existing parameter set a number of ways. Once a parameter set is recalled, the text window displays the retrieved acquisition and processing parameters for the set in the text output window.

Using GLIDE

GLIDE can also be used to retrieve data. However, use this method to retrieve only data on parameters and FIDs. Perform the following steps to retrieve data with *GLIDE*:

1. Activate *GLIDE* by clicking the **GLIDE** button in the Main Menu.
2. Click on **Recall**.
3. In the Recall Setup window, type the full path of the FID file that you want.
4. Click on **Retrieve**.

   The data file is recalled. If the data was acquired with *GLIDE*, the `.def` files are also recalled into *GLIDE*.

Using the CDE File Manager

This method can be used to retrieve data on parameters, FIDs, or shim files. To use this method, the `listenon` macro must be, or must have been, executed. If file retrieval is a regular mode of operation, consider putting `listenon` in your local `login` macro. Do the following steps to retrieve data with CDE:

1. Start the CDE File Manager by using the CDE toolbar.
2. Go to the desired directory and double-click on the desired parameter, FID, or shim file.

   After you have selected the desired FID file, it is processed and displayed. `.def` files (files acquired with *GLIDE*) are retrieved into *GLIDE*.

Using the Menu System

1. Follow steps 1 to 4 above for listing parameter sets using the menu system. When the parameter set entries for the subdirectory you want are on view, as shown in step 4, highlight the parameter file you want, and click on **Return**.
2. Click on **Load**.

Using the Input Window

Enter the command **`rtp<(`*`directory`*`)>`**, where *`directory`* is the name of the directory containing the parameters set (e.g., to recall the standard proton parameters, enter `rtp('/vnmr/stdpar/H1')`). Note that adding the `.par` suffix is optional when using `rtp`).

After bringing parameters into the current experiment with `rtp` (or similar macros such as `rt`, `rtv`, and `convert`), the macro `fixpar` is automatically executed. This macro takes the following actions:

- Updates old parameter characteristics and reconciles parameter differences due to the hardware present on the spectrometer.
- Sets the `file` parameter and calls the `fixpar3rf`,`fixpar4rf`, and `fixpar5rf` macros to check for the existence of all acquisition parameters related to the third,

fourth, and fifth rf channels, respectively (if the channel exists on the system based on the value of the parameter `numrfch`). Any parameters found to be absent are created, characterized, and initialized by the appropriate macro.

- Checks if a macro `userfixpar` exists. If it does, `fixpar` runs that macro. This allows an easy mechanism to customize parameter sets.

The parameter `file` contains the file name of the parameter set returned by a `rt` or `rtp` macro. This parameter is reset when the `go` command is issued.

- If the system is not in automation mode (`auto='n'`), `file` is reset to `'exp'`.
- If the system is in automation mode (`auto='y'`), `file` is set to the path of the directory where the data is stored.

To Recall Standard Parameter Sets

The VNMR software offers several shortcuts if you only want to select standard parameter sets. Once a nucleus and solvent are selected, a parameter set is set up to do the experiment requested, complete with positioning of the transmitter and decoupler and, in the case of ^{1}H and ^{13}C, approximate referencing to TMS.

Using GLIDE

1. If the *GLIDE* interactive window is not open, open it entering **`glide`** in the input window or by clicking on the **GLIDE** button in the Main Menu.
2. Click on **Setup**.
3. Using the right mouse button, click on the triangle to the right of the Experiment entry in the window. A menu appears with choices such as `Proton 1D` and `Carbon 1D`.
4. Using the left mouse button, click on the experiment desired.
5. Using the right mouse button, click on the triangle to the right of the Solvent entry in the window. A menu appears with choices such as `CDCl3` and `Acetone`.
6. Using the left mouse button, click on the solvent desired.
7. Click on the **Setup** button at the bottom of the window.

Using the Menu System

1. Click on **Main Menu** > **Setup**.

   The Setup menu appears with the following buttons:

2. If you want ^{1}H or ^{13}C experiment with $CDCl_3$, click on **H1,CDCl3** or **C13,CDCl3**, as appropriate. Otherwise, click on **Nucleus,Solvent**.

   The Nucleus Selection menu appears with a choice of nuclei:

3. Click on the nuclei desired, or if the nucleus you want is not listed, click on Other to enter a different nuclei.

   The Solvent Selection menu appears with a choice of lock solvents:

4. Click on the solvent desired, or if the solvent you want is not listed, click on Other to enter a different solvent.

Using the Input Window and Menu System

1. Enter **`setup`** in the input window.

   The Nucleus Selection menu appears with a choice of nuclei:

2. Click on the nuclei desired, or if the nucleus you want is not listed, click on Other to enter a different nuclei.

   The Solvent Selection menu appears with a choice of lock solvent:

3. Click on the solvent desired, or if the solvent you want is not listed, click on Other to enter a different solvent.

Using the Input Window Only

- Enter the command **`setup(`*`nucleus`*`,`*`solvent`*`)`** where *`nucleus`* is chosen from among the nuclei for the files in the directory `/vnmr/stdpar`; typically `H1`, `C13`, `P31`, and `N15`, and *`solvent`* is chosen from among the solvents listed in the files in the directory `/vnmr/solvents`; typically `CDCl3`, `C6D6`, `D2O`, `DMSO`, `Acetone`, `CD2Cl2`, and `CD3OD`.

  For example, to set up parameters to do a carbon experiment with DMSO-d_6 as the solvent, enter `setup('C13','DMSO')`.

To Create Selected Parameters

For certain types of experiments, the `addpar` macro creates selected parameters to add to the current experiment.

Using the Input Window

- Enter the appropriate command to add parameters:

`addpar('2d')`	For a 2D experiment
`addpar('3d')`	For a 3D experiment
`addpar('3rf')`	For a 3rd rf channel
`addpar('4d')`	For a 4D experiment
`addpar('downsamp')`	For downsampling data
`addpar('fid')`	For a FID display
`addpar('image')`	For imaging
`addpar('ll2d')`	For 2D line listing
`addpar('lp')`	For linear prediction, acquisition dimension
`addpar('lp,1')`	For linear prediction, 1st implicit dimension
`addpar('lp,2')`	For linear prediction, 2nd implicit dimension

`addpar('oversamp')`	For oversampling data
`addpar('ss')`	For solvent suppression

With no argument specified, `addpar` displays instructions for its use. Refer to the description of `addpar` in the *VNMR Command and Parameter Reference* for a list of the parameters created with each `addpar` argument.

To List Parameter Groups

You can display various groups of parameters in the text window using the `dg` command or one of the macros `dg1`, `dg2`, `dgs`, and `dglp`: The string parameters `dg`, `dg1`, `dg2`, and `dgs` control which parameters are displayed by the macro with the same name as the parameter (e.g., *parameter* `dg` controls the parameter group displayed by *macro* `dg`). Text editors `paramvi(parameter)` or `paramedit(parameter)` are available for modifying the string parameters. Refer to the manual *VNMR User Programming* for details on how to modify the parameters.

Using the Input Window

- Enter the appropriate command or macro:

`dg`	Display group of acquisition and 1D/2D processing parameters
`dg1`	Display group of display parameters
`dg2`	Display group of third and fourth rf channels parameters (typically for the second and third decouplers, respectively) and 2D processing of 3D data sets parameters.
`dgs`	Display group of shims and automation parameters.
`dglp`	Display group of linear prediction parameters.

6.4 Removing and Inserting the Probe

If you want to use another probe or must remove the probe for cleaning, you need to know how to remove the probe and reinsert it. Since many types of probes are available, only general information is given here. Refer to the manual *NMR Probes Installation*. for more information on Varian probes.

To Remove the Probe

To remove the probe, you do not need to turn off the air supply or the transmitter.

1. If acquisition is in progress, stop the acquisition. Enter **`dm='n' su`**.
2. If a sample is in the probe, remove the sample.
3. Remove the cooling line from the blue nipple on the probe.
4. Remove the cables from the collar attached to the probe. Typically, there are cables for lock, observe, and decouple, and VT control. The VT cable is a 9-pin cable attached to a connector with steel screws or a steel clamp. If there are screws, carefully remove them with the small nonmagnetic screwdriver provided. If there is a clamp, squeeze the connector to unplug it.
5. Loosen the two knurled small bolts that hold the probe to the bottom of the magnet body, support the probe with one hand, and guide it slowly out of the magnet with

the other hand. As the probe begins its descent, remove the rubber VT connector from the glass protrusion on the rear of the probe.

To Insert the Probe

Reinsertion of the probe follows the reverse of the removal procedure above.

6.5 Using Probe Files and Templates

Table 12 summarizes the VNMR macros and parameters connected with probe files. Refer to the manual *Walkup NMR Using GLIDE* for more information on probe files.

Table 12. Probe File Macros and Parameters

Commands	
`addnucleus<(nucleus)>`	Add new nucleus to existing probe file
`addparams*`	Add parameter to current probe file
`addprobe<(probe_name<,'system'>)>`	Create new probe directory and probe file
`getparam(param<,nucleus>):$value`	Retrieve parameter from probe file
`setdecpars`	Set decoupler parameters values from probe file
`setdec2pars`	Set decoupler 2 parameters values from probe file
`setparams(param,value<,nucleus>)`	Write parameter to current probe file
`updateprobe*`	Update probe file
`* addparams(param,value,nucleus<,'tmplt'><,'system'>)`	
`updateprobe(<probe|'tmplt'><,"system'>)`	
Parameter	
`probe {string}`	Probe type

6.6 Tuning the Probe

Probe installation and tuning varies with the spectrometer and the type of probe. Table 13 summarizes the VNMR commands connected with tuning probes. Different NMR laboratories also have different standards about probe tuning.

Table 13. Probe Tuning Commands

Commands	
`btune`	Tune broadband channel on *GEMINI 2000*, any channel on *MERCURY*
`ctune`	Tune ^{13}C channel on ^{1}H/^{13}C *GEMINI 2000*
`dtune`	Tune lock channel on *GEMINI 2000*
`go*`	Submit experiment to acquisition
`htune`	Tune ^{1}H channel on *GEMINI 2000*
`qtune`	Graphical tuning tool on UNITY*INOVA* and UNITY*plus*
`sethw('tune',n)`	Place *GEMINI 2000* into tune mode
`su`	Submit setup experiment to acquisition
`tune*`	Assign frequencies on UNITY*INOVA* and UNITY*plus*
`tuneoff`	Turn off tuning mode on *GEMINI 2000*
`* go<(<'acqi><,'nocheck'><,'nosafe'>)>`	
`tune(freq1<,freq2,freq3,freq4>),tune(ch1,freq1<,chan2,freq2,.>)`	

Sample Changes

In general, if the probe is already tuned to the proper nucleus (as is almost always the case for proton and carbon observation), only a small amount is gained by tuning the probe to match your particular sample.

An exception to this rule occurs when switching from “normal” organic solvents to strongly ionic samples, such as a water solution with 1M buffer. If the probe is tuned for an organic solvent, such as $CDCl_3$, and a strongly ionic sample is then inserted, you may find a lengthening in the 90° pulse width by a factor of two or three.

For single-pulse experiments, this detuning of the probe will cause an apparent deterioration of signal-to-noise (since you will only be using a 30° pulse, for example, when you intended to use a 90° pulse) but in many cases this effect will be small.

Quarter-Wavelength Cable

When a large change is made in the frequency of the observe nucleus on broadband systems, such as switching from ^{13}C to ^{15}N, an additional change is made in the quarter-wavelength cable, a coiled cable located on the system as follows:

- Attached to the preamplifier housing for 500-, 600-, and 750-MHz systems.
- Attached to the inside of the left magnet leg on the *MERCURY-VX*, *MERCURY*, and *GEMINI 2000*.
- Attached to the inner face of the magnet console interface unit as part of the observe circuitry on other systems.

The quarter-wavelength cable is *not* changed for each nucleus, but only for broad ranges of frequencies (for example, 40 to 80 MHz), usually covering a factor of two (an octave) in frequency. An incorrect cable does not typically affect signal-to-noise, but may have a profound effect on the 90° pulse length.

To Tune Probes on UNITY*INOVA* and UNITY*plus*

Probes on UNITY*INOVA* and UNITY*plus* systems can be tuned through the TUNE INTERFACE panel or the graphical probe tuning program `qtune`.

Using the TUNE INTERFACE Panel

Probes can be tuned using a special panel called the TUNE INTERFACE, shown in Figure 22. The panel is located either on the magnet-console interface or on the dual-preamplifier assembly. The panel contains the following displays, readouts, and ports:

- At the top of the panel is the TUNE INTERFACE display, a rectangular liquid-crystal display that shows a numerical value two ways—as a digital readout in the center of the display and as an analog representation along the oval surrounding the digital readout.

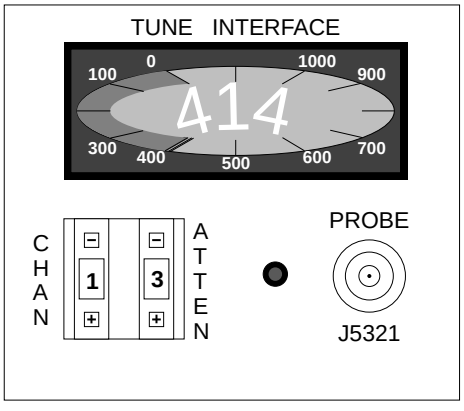


Figure 22. TUNE INTERFACE Panel

- Below the display are two single-digit readouts labeled CHAN and ATTEN. The CHAN readout can be set to 0 for OFF or to the channel being tuned (1, 2, 3, etc.), and the ATTEN readout is the amount of attenuation (analogous to the TUNE LEVEL knob on older systems). The attenuation is selected in units of 10 dB. The maximum attenuation is 79 dB, which is selected by a setting of 8. Above and below each readout are buttons for setting the value of the readout.
- At the lower right of the panel is a red indicator light and a BNC probe port labeled PROBE J5321.

Tuning a probe on a UNITY*INOVA* or UNITY*plus* system using the TUNE INTERFACE panel takes the following steps:

1. Set up the spectrometer to observe the nucleus of interest.

   Often, the system is already set to the correct nucleus; if not, proceed as if you were setting up an experiment (see Chapter 7, “Acquiring Data,” for information).

2. Using the appropriate procedure given below for your system, change the rf cable attached to the probe channel you plan to tune. No filters should be in-line during the tuning procedures:
   - UNITY*INOVA* and UNITY*plus* 200, 300, or 400 systems: Disconnect the cable from the H Band CM or the B Band CM port at the rear of the magnet-console interface. Connect this cable to the PROBE J5321 port on the TUNE INTERFACE panel.
   - UNITY*INOVA* and UNITY*plus* 500, 600, or 750 systems: Disconnect the cable from the PROBE J5311 port on the broadband preamplifier or the $^{1}H/^{19}F$ J5301 port on the preamplifier. Connect this cable to the PROBE J5321 port on the TUNE INTERFACE panel. Then disconnect the cable from the OUTPUT port (J5312 or J5302) and connect it to the TUNE OUTPUT J5323 port.

3. Two methods are available to set the tune frequency. Until you set up the tune frequencies with one of the methods (`su` or `tune`), the TUNE INTERFACE panel will not work after powering on or after resetting the acquisition console.
   - The first method is to enter `go` or `su`. Each time `go` or an `su` executes, the console receives a frequency for each channel defined for the experiment. This frequency also becomes the one used during tune. The table below shows the relationships between the channel selected and the associated parameters:

Channel 1	`tn`	`sfrq`	`tof`
Channel 2	`dn`	`dfrq`	`dof`
Channel 3	`dn2`	`dfrq2`	`dof2`
Channel 4	`dn3`	`dfrq3`	`dof3`

     For descriptions of these parameters, refer to the *VNMR Command and Parameter Reference*.
   - The second method is to enter `tune`. Refer to description of `tune` in the *VNMR Command and Parameter Reference* for details. The settings remain in effect until the next `go` or `su` command executes. The `tune` command is available on UNITY*INOVA* and UNITY*plus* systems only.

4. Press the CHAN buttons until the readout is the number of the rf channel you want to tune. Start with channel 1.

   This turns on the tuning function for the channel. The TUNE INTERFACE display should shows a number, and the red indicator light should not flash. (If the light flashes, check the connector to the cable for an improper connection.)

5. Press the ATTEN buttons until the readout is 6, 7, or 8.
6. If necessary, insert the appropriate sticks into the probe. Refer to the probe installation manual as to which sticks are needed to tune to the desired nucleus.
7. Tune the probe. As the probe gets closer to being tuned, the number on the TUNE INTERFACE display will decrease.
8. Press the ATTEN button until the readout is 8, to increase the tuning level sensitivity. Continue tuning until the number displayed on the TUNE INTERFACE display is as close to zero as possible.
9. Disconnect the tuning function by pressing the CHAN buttons until the readout is 0. (During normal spectrometer operation, CHAN must be set to 0 or acquisition will *not* be allowed.)
10. Reconnect the rf cables to their original position as follows:
    - UNITY*INOVA* and UNITY*plus* 200, 300, or 400 systems: Disconnect the cable from PROBE J5321 port on the TUNE INTERFACE panel. Connect the cable to the H Band CM or the B Band CM port at the rear of the magnet-console interface.
    - UNITY*INOVA* and UNITY*plus* 500, 600, or 750 systems: Disconnect the cable from PROBE J5321 port on the TUNE INTERFACE panel. Connect this cable to the PROBE J5311 port or the $^{1}H/^{19}F$ J5301 port, whichever was the original port. Then disconnect the cable to the TUNE OUTPUT J5323 port and connect it to the OUTPUT port (J5312 or J5302, as appropriate).

    At this time, the red indicator light should turn off.
11. Repeat the steps above for each channel on the system.

For further information about probe installation and tuning on the UNITY*INOVA* and UNITY*plus*, refer to the manual *NMR Probes Installation*.

Using the Graphical Probe Tuning Program (qtune)

This section describes how to use the graphical probe tuning program, `qtune` (shown in Figure 23), for swept-tune-type NMR probe tuning. `qtune` is available on UNITY*INOVA* and UNITY*plus* systems.

`qtune` runs on the host computer and offers you an interactive tuning method that provides separate information for matching and resonant frequency. This program is especially useful for tuning probes with complicated coil configurations, such as imaging probes.

After the system is put into tune mode, the reflected power from the probe passes through the directional coupler and is detected and digitized by the receiver circuitry: Any power that the receiver detects is reflected power. Taking one (or more) complex pair of data points at each frequency gives a data set that shows reflected power versus frequency. A coil tuned to a specific frequency (usually the frequency of the nucleus the user wants to observe) reflects little power at that frequency. The acquisition system then sweeps through the desired frequency range and gathers data on reflected power interactively. The user can adjust certain parameters interactively during the experiment.

To Tune a Probe with qtune

This procedure describes how to use the `qtune` program to tune an NMR probe.

1. Set up the system for tuning:

   UNITY*INOVA* and UNITY*plus* – leave the switch set to observe mode.

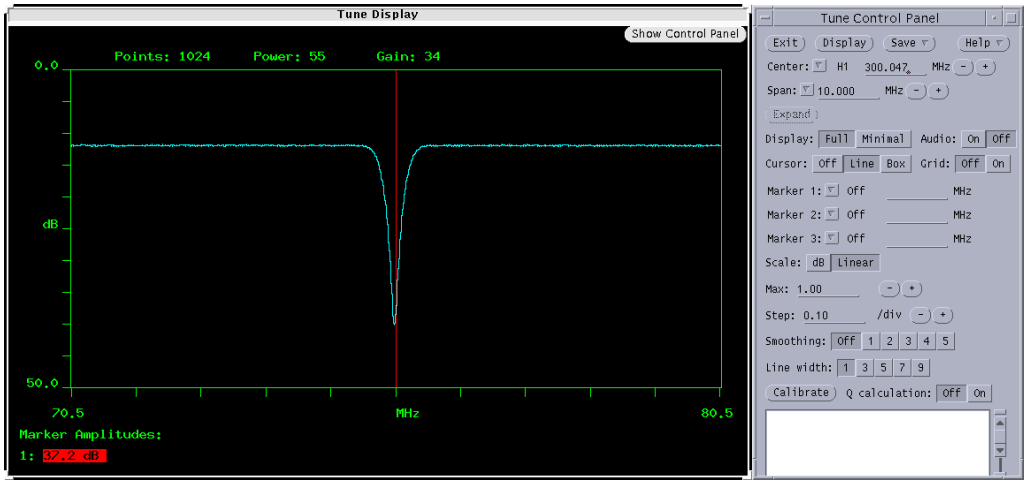


Figure 23. Probe Tuning Window (`qtune` Program)

MERCURY-VX – connect the following cables:

- Connect the appropriate cable from the probe (J5102 or J5302) to the TUNE J5402 connector on the inside of the magnet leg.
- Connect the appropriate cable from the transmitter (J5602 or J5603) to the TUNE J5604 connector.
- Connect the appropriate cable from the receiver (J5303 or J5103) to the Q TUNE J5403 connector.
- Enter **`tn='`*`n`*`' su`**, where *n* is the nucleus to be tuned (e.g. `tn='H1'`).

2. In the VNMR input window, enter **`qtune(`*`gain`*`,`*`power`*`)`**, where *`gain`* and *`power`* are appropriate gain and power values. Typical entries are `qtune(20,65)` for UNITY*INOVA* and UNITY*plus*, and `qtune(0,15)` for *MERCURY-VX*. Generally you want as low a gain value as possible with as high a power value as possible. If `qtune` is entered without arguments, the default values of 50 for `gain` and 60 for `power` are used.

   The Tune Display and Tune Control windows open, similar to Figure 23. The Tune Display is centered on the resonant frequency of the current experiment (`sfrq`).

   To change the gain and power values, click Exit in the Tune Control Panel and reenter the `qtune` command with more appropriate values.

3. In the **Display** field, select **Full** or **Minimal**.
   - Full display shows the network-analyzer-like graph, as shown in Figure 23.
   - Minimal display simplifies the tune display by showing numerical values instead of the graph, as shown in Figure 24. When sweeping over a range of frequencies, the minimal display shows minimum reflected power and center frequency. When in CW mode, the minimal display shows the average reflected power and the current frequency. Several display controls on the Tune Control Panel are disabled in minimal display mode, including cursors, grid, and markers.

4. In the **Audio** field, select **On** or **Off**.

   If set to On, a volume slider becomes available and a sound is generated that indicates how close the minimum reflection is to the center of the sweep window—

Figure 24. Minimal Display Mode for the Tune Display

the lower the pitch of the sound, the closer the minimum reflection is to the center. The sound immediately stops if the response lacks a discernible minimum reflection or if CW mode is set

To use the audio capability requires:

- An audio speaker on the Sun computer.
- The probe tuned well enough so that a clearly discernible minimum reflection exists in the signal.
- A range of frequencies sent to the probe (i.e, audio requires sweep mode rather than CW mode).

5. Place a marker on the resonant frequency to which you want to tune the probe as follows (this option is not available in minimal display):

   a. In the Tune Control Panel (see Figure 25), click on the triangle next to one of the markers to open a pull-down menu (Figure 29 shows the Marker 1 menu).

      For more detail on using markers, see the “To Use Cursors, Grid, and Markers” on page 120.

   b. In the menu, select the resonant frequency to which you are tuning the probe.

      A marker corresponding to the selected frequency appears in the Tune Display window.

6. In the Tune Control Panel, type values as appropriate in the **Span**, **Scale**, and other fields on the Tune Control Panel.

   Using the dB scale usually facilitates probe tuning. See the “To Adjust the Span” on page 120.

7. Adjust the tune and match capacitors while watching the Tune Display window. Use the match capacitor to increase the depth of the dip as much as possible. Use the tune capacitor to center the dip on the marker created in step 5.

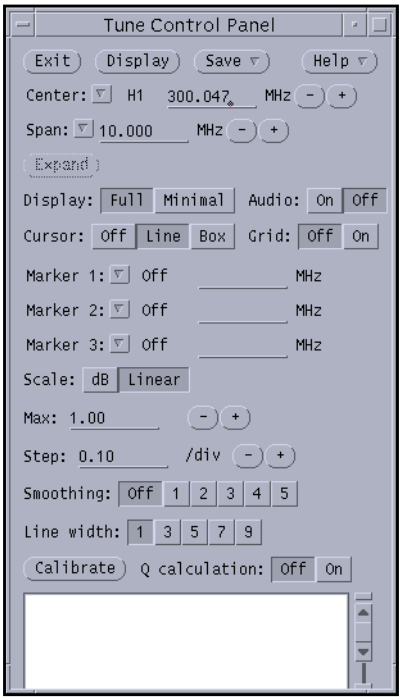


Figure 25. Tune Control Panel (`qtune` Program)

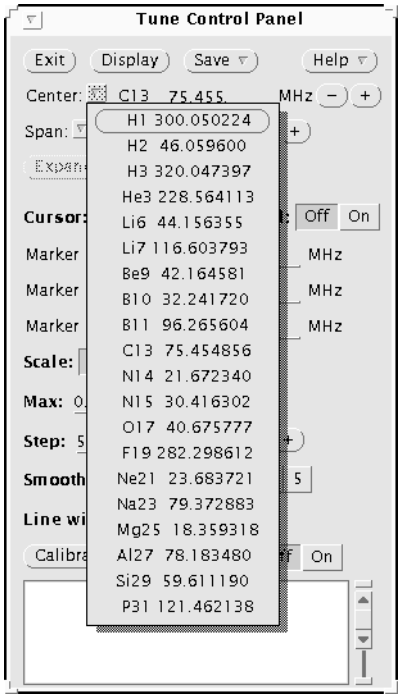


Figure 26. Pull-Down Menu for Center Frequencies

The dip displayed in the Tune Display window shows where little power is reflected at the frequency being observed. The depth of the peak shows the accuracy of the impedance matching of the probe coil to the transmitter and receiver. The horizontal location of the dip shows the frequency at which little power is reflected. The goal of probe tuning is to increase the depth of the peak (matching) while centering the dip at the desired frequency.

8. After the probe is tuned, click **Exit**. You are ready to begin the experiment.

To Select a Center Frequency

The center frequency is the resonant frequency to which the probe is to be tuned. A list of center frequencies appears in the Center pull-down menu in the Tune Control Panel (see Figure 26). This list of frequencies is read from the VNMR `nuctable` file.

Note that any frequency you type into the field will not be read until you press Return. This applies to all text entry fields.

1. In the **Center** field, click on the triangle to open the pull-down menu, then select a frequency that equals or is close to the frequency you want.
2. Adjust the frequency by typing a new value in the Center field or by clicking the – and + buttons.

The – or + buttons decrease or increase the value by the width of one span.

If the center frequency is either typed in or changed by the – or + button, user is displayed next to the frequency. If the typed value happens to correspond to a nuclear frequency in the pull down menu, that nucleus is displayed.

If the new center is too close to either of the system frequency limits, the span is decreased to allow the new center to be accepted, the message window will beep, and an error message will appear. If the specified center is past either frequency limit, the message window will beep, and an error message will appear.

To Adjust the Span

The span is the sweep width, in MHz, used in the Tune Display.

1. To decrease or increase the span to the next in the series 1,2,5 10,20, etc., in the **Span** field, enter a value or click the – or + button.

   Setting the span to less than 1000 Hz causes the message window to beep and an error message to appear.

   Setting the span to more than maximum span causes the message window to beep and an error message to appear.

   Setting the span to a value beyond the maximum or minimum frequencies causes the span to decrease, the message window to beep, and user warnings to appear.

2. In the **Span** field, click on the triangle to open the Span pull-down menu (see Figure 27).

   - Select **Last Span** to return to the previous span value
   - Select **Maximum Span** to make the spectrometer sweep from the minimum to maximum allowable frequencies.
   - Select **CW** to temporarily stop frequency sweeping and to make the transmitter put out a CW signal. This sets the frequency to the currently selected center frequency. This mode is useful for checking the reflected power on the tune meter or for making other tests that require a fixed frequency.

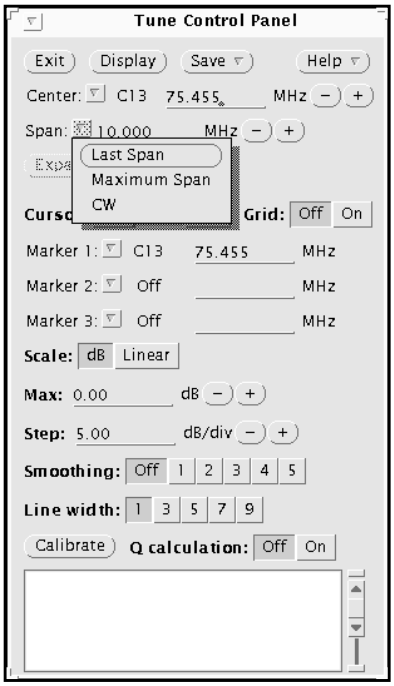


Figure 27. Pull-Down Menu For Span

To Use Cursors, Grid, and Markers

Cursors and markers appear on the Tune Display and are used the same way they are used in VNMR. Cursors and markers are color coded and the frequency positions of each are displayed on the bottom of the Tune Display. Cursor, grid, and marker controls are not available in minimal display.

Cursors – In the **Cursor** field, the Tune Control Panel provides three cursor modes (see Figure 28)

Figure 28. Cursor and Grid Controls

- Select **Off** to turn cursors off so that no cursors are displayed.
- Select **Line** to display a single cursor that specifies one frequency. The frequency position of the cursor and the signal amplitude at that frequency are displayed on the bottom of the Tune Display window.
- Select **Box** to display two cursors for use with the Expand button (for setting the span to a narrower range). After a region is expanded, the cursor mode switches back to the

Off mode. The frequency positions of the cursors, as well as the delta and the signal amplitudes, are displayed on the bottom of the Tune Display window.

Grid – In the **Grid** field, select **Off** or **On** (see Figure 28) to control a grid display in the Tune Display window. The grid helps in reading the reflected power levels off of the graph. The grid does not slow down the drawing time of the graph.

Markers – In the **Marker 1**, **Marker 2**, and **Marker 3** fields, the Tune Control Panel provides three markers for marking fixed frequencies. Each marker has a pull-down menu (see Figure 29) that lists the same nuclear frequencies and the Center pull-down menu. Each marker also has an entry field for entering a frequency.

You can use markers for observing fixed frequencies, for example the two nuclear frequencies of a double tuned probe. You can then vary the span, and the markers will appear and disappear, depending on whether their frequencies are being scanned in the current experiment.

Attempting to set the markers to values beyond the system frequency limits causes the message window to beep and produces an error message.

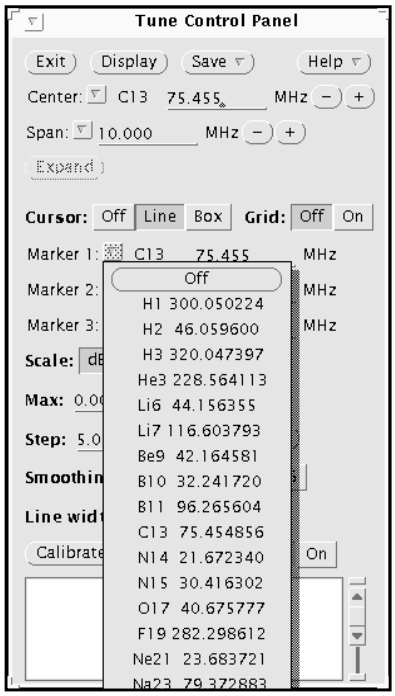


Figure 29. Pull-Down Menu for Marker 1

To Change the Vertical Scale

You can change the vertical scale of the Tune Display window by selecting whether the data is scaled in a linear or logarithmic manner (see Figure 30).

1. In the **Scale** field, the Tune Control panel provides two scaling modes:
   - Select **dB** to provide a logarithmic scale in units of dB.
   - Select **Linear** to a linear scale with arbitrary units.

   The dB scale shows a deeper dip for more accurate match adjustment.

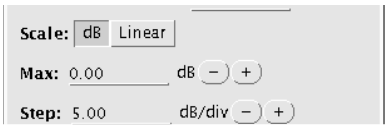


Figure 30. Scale Controls

2. In the **Max** field, type a value you want for the top line in the Tune Display.

   Setting a Max value beyond system limits generates a beep and an error message.

3. In the **Step** field, type a value you want for the number of units per division mark of the current scale (dB or linear) on the *y* axis of the Tune Display.

   Step helps by making the height of a probe resonance appear larger or smaller.

   Setting a Scale value beyond system limits generates a beep and an error message.

Q Calculation

Probe Q factor determines sensitivity. Q is defined as the frequency of the resonant circuit divided by the half power bandwidth.

1. Near the bottom of the Tune Control Panel, select Q calculation: On.

The current Q value and resonant frequency appears at the top of the Tune Display window, and a horizontal cursor appears on the plot.

2. In the Tune Display window, use the middle mouse button to place the horizontal cursor on the base line (reflected power level outside of the resonance line). The Q calculation appears at the top of the Tune Display window.

The Q that is shown is determined as follows:

- The software finds the lowest point on the display and designates this as the resonance. The frequency displayed is, at best, only as accurate as the frequency difference between points. You must take this into account when quoting Q measurements.
- This lowest point is used as V_{min}. The software takes the level of the horizontal cursor as the baseline, or V_{max}.
  V_{max} is assumed to be a frequency where all the rf energy is reflected by the probe.
- The two frequencies that have the signal level of Equation 1 are ω_1 and ω_2.

$$\frac{V_{max}}{\sqrt{5}} \qquad \text{[Eq. 1]}$$

- Q is calculated from Equation 2, where ω_r is the resonant frequency

$$Q = \frac{\omega_r}{|\omega_1 - \omega_2|} \qquad \text{[Eq. 2]}$$

- The software checks that the low point (the bottom of the dip) is at least 15 dB below the baseline. If this is not true, the calculated Q value is not accurate, and is, therefore, not reported (the string `"- - -"` appears in the Q value field). The resonance frequency, however, is still given.

Calibrating the Tune System

A Tune Calibration window is available for calibrating the tune system using a shorting load, an open load (no device attached), and a 50-ohm load.

To calibrate the tune system.

1. Set up the system for tuning:

   UNITY*INOVA* UNITY*plus* – Leave the switch set to observe mode.

   MERCURY-VX – Connect the following:

   - Connect the appropriate cable from the probe (J5102 or J5302) to the TUNE J5402 connector on the inside of the magnet leg.
   - Connect the appropriate cable from the transmitter (J5602 or J5603) to the TUNE J5604 connector.
   - Connect the appropriate cable from the receiver (J5303 or J5103) to the Q TUNE J5403 connector.
   - Enter **`tn='`*`n`*`' su`**, where *n* is the nucleus to be tuned (e.g., `tn='H1'`).

2. Click the **Calibrate** button on the Tune Control Panel. The Tune Calibration window opens (see Figure 31).

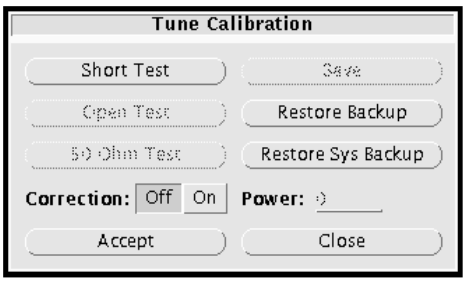


Figure 31. Tune Calibration Window

You must run the calibration tests in the following order:

- Short Test
- Open Test
- 50 Ohm Test

The test buttons are only available in this order.

The program stores only correction coefficients in files. Therefore, you will not be able to view old calibration sweeps after the experiments are finished.

3. In the **Correction** field, select **Off** or **On** to disable or enable calibration corrections, respectively. The default is enabled.

   If valid calibration files are not present, this button is not available.

4. Connect a shorting load:
   - UNITY*INOVA* and UNITY*plus* – Connect a shorting load to the tune port.
   - *MERCURY-VX* – Connect a shorting load to TUNE J5402 on the inside (probe side) of the magnet leg.
5. Click the **Short Test** button.
6. Remove the shorting device from the tune port.
7. With no load on the tune port, click the **Open Test** button.

   The program divides the full range of the spectrometer into 32 frequency bands and runs 32 experiments. This data is merged into one high-resolution data set. After enough data are collected, the Accept button becomes available. If ADC overflow occurs, a warning message appears.
8. After you see a strong signal (the signal will be stronger at low frequencies than at high frequencies) that does not cause ADC overflow, click the **Accept** button.
9. Attach a 50-ohm load:
   - UNITY*INOVA* and UNITY*plus* – Connect the 50-ohm load to the tune port.
   - *MERCURY-VX* – Connect the 50-ohm load to TUNE J5402 on the inside (probe side) of the magnet leg.
10. Click the **50 Ohm Test** button.

    The program divides the full range of the spectrometer into 32 frequency bands and runs 32 experiments. The data is merged into one high-resolution data set. After enough data are collected, the Accept button becomes available. If ADC overflow occurs, a warning message appears.
11. Click the **Accept** button and remove the 50-ohm load from the tune port.
12. After all three tests are finished, click the **Save** button.

    The old calibration files are moved to `.bak` files, and new calibration files `std_ed.cal`, `std_es.cal`, and `std_er.cal` are calculated. These files are stored in `$vnmrsystem/tune/tunecal`. If the files cannot be saved, the program produces a beep and an error message.
13. Click the **Close** button.

To Restore the Previous Calibration File

If you have an incorrect calibration file and do not want to re-run the calibration tests, restore the previous calibration files:

1. Click the **Calibrate** button on the Tune Control Panel. The Tune Calibration window opens (see Figure 31).
2. Click the **Restore Backup** button.

The program replaces the new calibration files with the `.bak` files. If the program does not find all of the backup files, an error message appears.

To Restore the Original Calibration Files

System backup files can be installed by copying the following `.cal` files on top of the corresponding `.sys` files:

- `std_ed.cal` to `std_ed.sys`
- `std_es.cal` to `std_es.sys`
- `std_er.cal` to `std_er.sys`

To restore these system calibration files, click the Restore Sys Backup button. The program replaces the new calibration files with the `.sys` calibration files created at system installation.

Online Descriptions of the Tune Control Panel

To get on-line descriptions of the buttons and fields in the Tune Control Panel, click the **Help** button with the right mouse button. A pull-down menu similar to that shown in Figure 32 appears. Select the topic of interest from the menu.

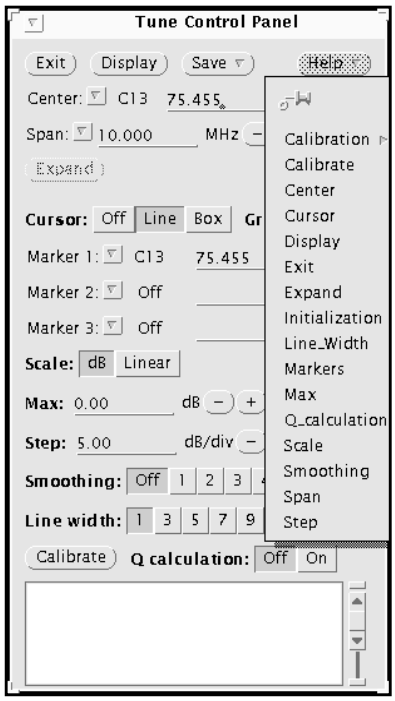


Figure 32. Help Pull-Down Menu

Tuning Probes on *MERCURY-VX*, *MERCURY*, *GEMINI 2000*

For *GEMINI 2000* systems, the `btune`, `ctune`, `dtune`, `htune`, and `tuneoff` macros turn rf on and off at the transmitter boards for tuning. *MERCURY-VX* and *MERCURY* use only `btune` and `tuneoff`. None of these macros use arguments.

- On *MERCURY-VX*, *MERCURY*, and *GEMINI 2000* broadband systems, `btune` turns on the broadband transmitter, directing about 0.5 watts of rf at frequency `sfrq` + `tof` to the probe. Before using `btune`, switch the cable on the magnet leg. `tuneoff` turns off the transmitter.
- On *GEMINI 2000* $^{1}H/^{13}C$ systems, `htune` turns on the ^{1}H transmitter, directing about 0.5 watts of rf to the probe. `tuneoff` turns off the transmitter. Similarly, `ctune` turns on the ^{13}C transmitter, directing 0.5 watts of rf to the probe, and `tuneoff` turns off the transmitter.

CAUTION: **Only qualified service personnel should tune the lock channel. An incorrectly tuned lock channel can damage equipment and cause erratic results.**

- On all *GEMINI 2000* systems, `dtune` turns on the lock (^{2}H) transmitter for tuning the lock channel.
- On all *GEMINI 2000* systems, the macro `sethw('tune',n)` is used internally by `btune` (`n` is 4 or 5), `ctune` (`n` is 2), `dtune` (`n` is 3), `htune` (`n` is 1), and `tuneoff` (`n` is 0 or 6). `sethw` is not normally entered by the user directly.

The procedures below are typical in tuning a *GEMINI 2000* probe. For further information, refer to the manual *NMR Probes Installation*.

Observe Coil Tuning on MERCURY-VX, MERCURY, BB GEMINI 2000

This example shows how to tune to ^{13}C. To tune to another nucleus, enter the name of that nucleus instead of `'C13'` in step 1.

1. Join an appropriate experiment and enter `tn='C13' su`.
2. Move the cable from the ^{13}C connector (J5302) to the TUNE connector (J5402).
3. Move the cable from the ^{13}C connector (J5603) on the rear of the magnet leg to the TUNE connector (J5604) just above it.
4. Enter `btune`.
5. Turn the meter switch to the TUNE position.
6. Adjust the TUNE control knob for a mid-range reading.
7. Turn the observe coil tuning rod until the meter reaches a minimum reading.
8. Turn the observe coil matching rod for a minimum meter reading. Adjust the TUNE knob if needed.
9. Switch back and forth between the observe coil tuning rod and the observe coil matching rod until you achieve an absolute minimum meter reading. Once a minimum is obtained, enter `tuneoff`.

   If the tuning is far off, it may be better to turn each rod past the minimum meter reading before turning the other rod.
10. Return the two cables to their original positions and turn the meter switch to SPIN.

Decoupler Coil Tuning on MERCURY-VX, MERCURY, BB GEMINI 2000

CAUTION: **Before tuning the decoupler coil, check that air is flowing through the probe dewar and decoupler cooling line, cooling both the sample and decoupler coil. Excessive heat will damage the sample and the decoupler tuning capacitors. During VT operation, the probe dewar requires nitrogen for cooling. For maximum power, use at least 20 CFH or 9.5 LPM.**

1. Join an appropriate experiment and then enter `tn='H1' su` (for ^{1}H) or `tn='F19' su` (for ^{19}F).
2. Move the proton probe cable from the ^{1}H connector (J5102) on the magnet leg to the TUNE connector (J5402).
3. Move the proton cable in the rear of the magnet leg to the coaxial tuning jack labeled TUNE J5604.
4. Enter `btune`.
5. Turn the meter switch to the TUNE position.
6. Adjust the TUNE control knob for a mid-range reading.

7. Turn the decoupler coil tuning control to obtain a minimum tuning meter reading. Adjust the TUNE knob as needed. Once a minimum is obtained, enter `tuneoff`.
8. Return the two cables to their original positions and turn the meter switch to SPIN.

Proton Observe/Decoupler Coil Tuning on $^{1}H/^{13}C$ GEMINI 2000

1. Join an appropriate experiment and enter `tn='H1' su`.
2. Move the proton cable from the ^{1}H connector (J5102) on the magnet leg to the TUNE input connector (J5402), also on the magnet leg.
3. Move the proton cable in the rear of the magnet leg from the ^{1}H connector (J5602) to the TUNE connector (J5604).
4. Enter `htune`.
5. Turn the meter switch to the TUNE position.
6. Adjust the TUNE control knob for a mid-range reading.
7. Turn the proton coil tuning rod for a minimum meter reading. Adjust the TUNE knob if needed. Once a minimum is obtained, enter `tuneoff`.
8. Return the two cables to their original positions and turn the meter switch to SPIN.

Carbon Observe Coil Tunning on $^{1}H/^{13}C$ GEMINI 2000

1. Join an appropriate experiment and enter `tn='C13' su`.
2. Move the cable from the ^{13}C connector (J5302) to the TUNE connector (J5402).
3. Move the cable from the ^{13}C connector (J5603) on the rear of the magnet leg to the TUNE connector (J5604) just above it.
4. Enter `ctune`.
5. Turn the meter switch to the TUNE position.
6. Adjust the TUNE control knob for a mid-range reading.
7. Turn the ^{13}C coil tuning rod until the meter reaches a minimum reading.
8. Turn the ^{13}C coil matching rod for a minimum meter reading. Adjust the TUNE knob if needed.
9. Switch back and forth between the ^{13}C coil tuning rod and the ^{13}C coil matching rod until you achieve an absolute minimum meter reading. Once a minimum is obtained, enter `tuneoff`.

   If the tuning is far off, it may be better to turn each rod past the minimum meter reading before turning the other rod.
10. Return the two cables to their original positions and turn the meter switch to SPIN.

Tunning Probes on UNITY and VXR-S Systems

For UNITY and VXR-S systems, refer to the manuals that accompanied the system or the probe for the information you need.

6.7 Spinning the Sample

On the UNITY*INOVA*, *MERCURY-VX*, UNITY*plus*, UNITY, and VXR-S systems, and on *MERCURY* and *GEMINI 2000* with spinner control, when a sample is inserted, the last entered spin rate is used to regulate sample spinning. The actual spin rate is indicated three ways:

- In the LOCK display of the Acquisition window (`acqi` program), the actual spin rate is shown below the lock signal (in green type if regulated, in yellow if not regulated, or in red if off), see Figure 33.
- In the Acquisition Status window (`acqstat` program), the actual rate is given as well as a spin regulation indication.
- In the remote status unit (optional on systems other than *MERCURY-VX*, *MERCURY*, and *GEMINI 2000*) or on the magnet leg on the *MERCURY-VX*, *MERCURY*, and *GEMINI 2000*, the spin rate is shown by the spin light:

  If light is off, the sample is not spinning.

  If light is blinking, the sample is spinning but not at the last requested rate.

  If light is steady, the spin rate is being regulated at the last requested rate.

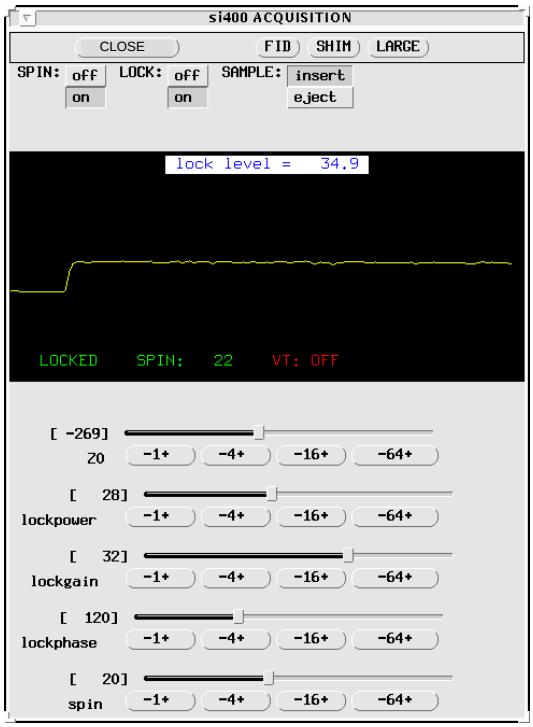


Figure 33. Spin Information in LOCK Display (`acqi` Program)

On *MERCURY* and *GEMINI 2000* systems without spinner control, the spin rate is controlled by adjusting the needle valve on the magnet leg. Spinning is indicated by a spin light and a needle valve on the magnet leg.

You can adjust spin rate from the input window or the Acquisition window. Typical spin rates are 15 for 10-mm tubes and 20–26 for 5-mm tubes.

The Spinner Control window (`spinner` program) provides spin speed control, experiment control, and low-speed or high-speed spinner selection, see Figure 34.

Table 14 lists commands and parameters related to adjusting sample spinning.

Using the Input Window

The `spin` *command* regulates sample spinning according to the `spin` *parameter* (note there is a `spin` command and a `spin` parameter). The `spin` command also sets rf frequency, decoupler status, and temperature. The value of the `spin` parameter is changed when a sample is inserted or one of the commands `spin`, `go`, `ga`, `au`, or `sample` is entered. Thus, the value of `spin` is not necessarily the current experiment. The `dgs` macro displays the group of shim and automation parameters, including `spin`. The spin

Table 14. Sample Spinning Commands and Parameters

Commands	
`acqi*`	Open the Acquisition window
`acqmeter<('host')>`	Open the Acqmeter window
`dgs`	Display group of shim and automation parameters
`spin`	Submit a spin setup experiment
`spinner`	Open the Spinner Control window
`* acqi<('par'|'disconnect'|'exit'|'standby')><:ret>`	
Parameters	
`in {'n','w','y'}`	Lock and spin interlock
`spin {0, 5 to 39, 'n'}`	Sample spin rate

speed can also be made a part of the standard parameter set for a given nucleus (this is covered later).

Applies to all systems if the optional spin control hardware is installed.

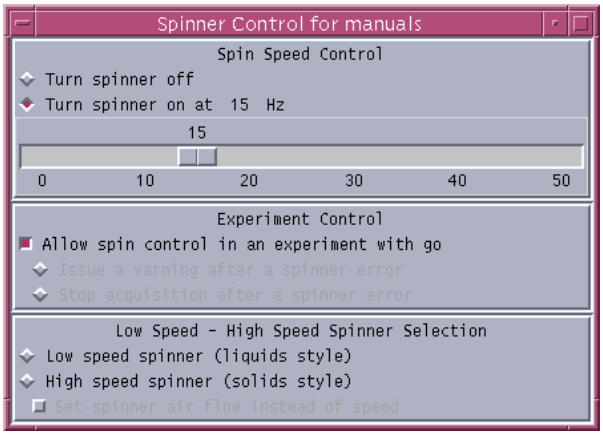


Figure 34. Spinner Control Window (`spinner` Program)

- Enter `spin=# spin`, where # is the desired spin rate. For example, entering `spin=15 spin` adjusts the spin rate to 15.

  If `spin` is set to a particular value and the interlock parameter `in` is set to `'y'`, spinning regulation is checked after each transient. Acquisition is aborted with an appropriate error message if spinning goes out of regulation, just as it does if lock is lost. If `in` is set to `'w'`, a warning is generated if the spin speed goes out of regulation; however, acquisition is not stopped. If `in` is set to `'n'`, spinning is checked and regulated before the first transient and not checked thereafter.

  The `spin` *parameter* can also be set to `'n'`, which indicates that no spin rate adjustment is to be done when acquisition begins. The system will still attempt to regulate at the last entered spin rate, but acquisition will not wait for regulation to occur. If `spin='n'` and `in='y'`, only lock loss causes acquisition to stop.

  The `in` parameter can be set to handle both lock level and spinner speed errors. For details, see “Lock Level and Spin Speed Error Handling” on page 150.

Using the Acquisition Window

Applies to all systems configured for acquisition if the optional spin control hardware is installed. This feature is not available on data stations.

1. If the Acquisition window is not open, enter `acqi` in the input window, then click on the Connect button in the window when it appears.
2. Click on the LOCK button.

The LOCK display appears with the following spin-related information, see Figure 33:

- The SPIN menu (near the top of the display)
- A readout of the actual spinning speed (at the bottom of the graphics window)
- Controls for changing the value of the `spin` parameter (at the bottom of the display)

The controls for changing `spin` consist of a readout with the current value of `spin` (shown in square brackets, e.g., `[ 20]`), a slide control for adjusting the value of `spin`, and four buttons (labeled –1+, –4+, –16+, and –64+) also for adjusting the value of `spin`.

3. Check that the on button in the SPIN menu is selected. Also check the current spinning speed displayed near the center of the LOCK display.
4. To adjust the `spin` parameter, use either of these methods:
   - Drag the mouse cursor across the slide control with the left button of the mouse held down. The value changes proportionally as the mouse moves.
   - Click on the –1+, –4+, –16+, and –64+ buttons as required. Clicking on a button with the left mouse button decreases `spin` by the amount shown on the button; clicking with the right mouse button increases `spin` by the amount shown on the button.

   For further information, see the “LOCK Display” on page 151.

Using the Spinner Control Window

The `spinner` command opens the Spinner Control window for control of sample spinning, see Figure 34. From this window, the spinner can be started or stopped, and experiment control of spinning can be turned off. That way, if an experiment you just joined has the `spin` parameter set to a value other than the current spinning speed, and you forget to set `spin` to `'n'` and type `go`, the spin speed will not be changed.

On the UNITY*INOVA* system, high-speed, solids-style sample spinning and low-speed, liquids-style sample spinning are both under computer control. The `spinner` program can be used to select these spinner types.

1. Enter the command `spinner` in the input window.

   The Spinner Control window appears.
2. Set the desired spinning speed by clicking the diamond next to Turn Spinner On and enter the speed value in Hz.
3. To disable experimental control of spinning, click the button next to Allow spin control in an experiment with go. A button that is indented (and red) is selected.

   When experimental control of spinning is disabled, you can choose how spinner errors are handled by the system—a warning is issued or acquisition is stopped.
4. Select a spinner mechanism type, low-speed (liquids-type spinning), high-speed (solids-type spinning), or automatic spinner type selection.

   If you select high-speed, you can choose to set the spinner air flow instead of the speed.

   If you select the automatic spin selection, you must also enter threshold values that tell the system when to switch to solids-type spinning.

For the high speed spinner probes (e.g., MAS), the following safety measures have been implemented to prevent rotor and stator damage:

- The air flow selected from the spinner window is ramped to the new value at a safe rate.
- If the spinner speed drops to zero and the spin setting is nonzero, the air flow will be shut off. This measure prevents spinner runaway if the tachometer fails.
- If for some reason the spinning speed cannot be reached, the air flow will be shut off. This measure prevents the continued spinning of a crashed rotor with more air flow.

6.8 Optimizing Lock

Under computer control, the lock system maintains the frequency stability of the spectrometer as the static field generated by the superconducting magnet drifts slowly with time or changes due to external interference. Locking makes the resonance field of the deuterium in the deuterated solvent coincide with the lock frequency.

The lock level can be viewed using the Acquisition window or the Acqmeter window:

- To view the lock level in the Acquisition window, enter `acqi` in the input window, click on the Connect button in the window when it appears, and then click on the LOCK button. The LOCK display appears.
- To view the lock level with the Acqmeter window, enter `acqmeter` in the input window or `Acqmeter` in a UNIX shell. A window appears (shown in Figure 35) that begins showing the lock level. Clicking with the right mouse button inside the window opens a popup menu that allows you to display VT and spin information or open a properties window that allows you to alter the display (also in Figure 35).

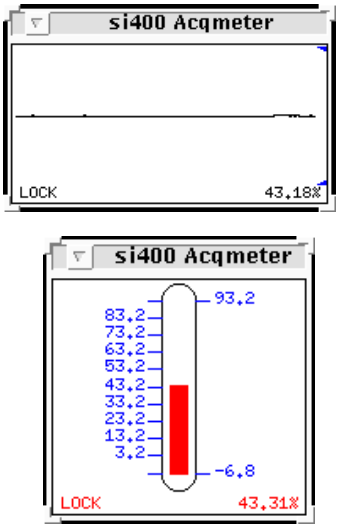


Figure 35. Acqmeter Lock Displays (`acqmeter` Program)

The entire lock optimization process can be skipped if optimum lock parameters are already known for a particular solvent and probe combination. Values for these parameters can be entered as part of a macro or using normal parameter entry (e.g., by entering `lockgain=30 lockpower=24`). These parameters do not take effect until an `su`, `go`, or equivalent command is given.

If automatic shimming is to be used, it is important to obtain an optimal lock signal. Manual adjustment often is done to achieve the maximum lock amplitude. This can result in a partly saturating condition, and a true non-saturating power is usually 6 to 10 dB lower. The response of the lock level is governed by the T_1 of the deuterated lock solvent as well as the magnet-determined or chemical exchange-determined T_2^* of the solvent. This T_1 can vary widely, from about 6 seconds for acetone-d_6 to about 1.5 seconds for $CDCl_3$ and lower for more viscous solvents. To allow a reliable, repeatable selection of lock power, automatic optimization may be used.

This section describes the lock parameters (`lockpower`, `lockphase`, and `lockgain`) and then describes methods of controlling lock. Lock loop time constant control is also described. Table 15 lists the lock commands and parameters discussed in this section.

Table 15. Lock Commands and Parameters

Commands	
`acqi*`	Open the Acquisition window
`acqmeter<('host')>`	Open the Acqmeter window
`lock`	Submit Autolock experiment
`readhw*`	Read acquisition hardware values
`sethw*`	Set acquisition hardware values (lock related)

`* acqi<('par'|'disconnect'|'exit'|'standby')><:ret>`
`readhw(par1,par2,...)<:val1,val2,...>`
`sethw(<'wait'|'nowait',>par1,val1<,par2,val2,...),`
`sethw('lock','on'|'off')`

Parameters	
`alock*`	Automatic lock status
`in {'n','w','y'}`	Lock and spin interlock
`lockacqtc*`	Lock acquisition time constant
`lockgain*`	Lock gain
`lockphase*`	Lock phase
`lockpower*`	Lock power
`locktc*`	Lock time constant
`shimset*`	Type of shim set
`z0*`	Z0 field position

`* alock {'y','n','a','auto','s','samp','u'} on` UNITY*INOVA;*
`alock {'y','n','a','s'} on` *GEMINI 2000*, *MERCURY-VX*, and *MERCURY*
`lockacqtc {1.2,4.7,12,48,in sec} on` UNITY*INOVA*;
`lockacqtc N/A on` *GEMINI 2000*, *MERCURY-VX*, and *MERCURY*
`lockgain {0 to 48 dB, 1-dB steps} on` UNITY*INOVA*;
`lockgain {0 to 30 dB, 10-dB steps} on` *GEMINI 2000*
`lockphase {0 to 360 degrees, in 1.4-degree steps}`
`lockpower {0 to 68 dB, 1-dB steps} on` UNITY*INOVA*;
`lockpower {0 to 40 dB, 1-dB steps} on` *MERCURY-VX* and *MERCURY*
`locktc {1.2,4.7,12,48,in sec} on` UNITY*INOVA*;
`locktc N/A on` *GEMINI 2000*, *MERCURY-VX*, and *MERCURY*
`shimset {1,2,3,...14} on` UNITY*INOVA*; `{1} on` *GEMINI 2000*
`shimset {1,2,3,...10}` on *MERCURY-VX*, and *MERCURY*
`z0 {–2048 to 2047, or –32768 to 32767}`

Lock Power, Gain, and Phase

Under computer control, lock power, gain, and phase are set by the lock parameters—`lockpower`, `lockgain`, and `lockphase`—with the following limits and step sizes:

- On UNITY*INOVA* and UNITY*plus*, lock power is 0 to 68 dB (68 is full power), lock gain is 0 to 48 dB, and lock phase is 0 to 360 degrees. Step size for power and gain is 1 dB; step size for lock phase is 1.4 degrees.

  On *MERCURY-VX* and *MERCURY*, lock power is 0 to 40 dB (40 is full power), lock gain is 0 to 39 dB, and lock phase is 0 to 360 degrees. Step size for power and gain is 1 dB; step size for lock phase is 1.4 degrees.

- On *GEMINI 2000*, lock power is 0 to 40 dB (40 is full power), lock gain is 0 to 30 dB, and lock phase is 0 to 360 degrees. Step size for power is 1 dB and step size for gain is 10 dB; step size for lock phase is 1.4 degrees.

- On UNITY and VXR-S, lock power is 0 to 63 dB (63 is full power), lock gain is 0 to 70 dB, and lock phase is 0 to 360 degrees. Step size for power and gain is 1 dB; step size for lock phase is 1.4 degrees.

On all systems except UNITY*INOVA*, *MERCURY-VX*, and *MERCURY*, and *GEMINI 2000*, setting lock power to 0 (`lockpower=0`) means no lock pulses, that is, no lock.

The Z0 field position parameter `z0` holds the current setting of the Z0 setting. The limits of `z0` are –2047 to 2047, in steps of 1, if the parameter `shimset` is set to 1, 2, or 10, and –32767 to +32767 if `shimset` is set to 3 through 9. On *MERCURY-VX* and *MERCURY* systems, `shimset` is 10. On *GEMINI 2000* systems, `shimset` is 1. Zero is no current.

The `readhw` command reads into VNMR the current values of lock system parameters in the acquisition hardware. To make VNMR set the lock values in the acquisition hardware, use the `sethw` command.

Lock Control Methods

A number of methods are available for controlling lock:

- Leave lock in the current state.
- Run an experiment unlocked.
- Use simple autolock.
- Use optimizing autolock.
- Perform full optimization of lock.

Each method is discussed in the following separate sections. Additional sections discuss error handling and lock loop time constant control.

Leaving Lock in the Current State

Using the Input Window

- Enter `alock='n'`
  If simple or optimized Autolock was previously selected, lock is established upon insertion of the new sample. If simple lock was previously selected, the system only locks if the new sample has the same lock solvent.

Running an Experiment Unlocked

Using the Input Window

Applies to all systems except *MERCURY-VX*, *MERCURY*, and *GEMINI 2000*.

- Enter `alock='u'`
  Lock is deactivated at the start of acquisition.

Simple Autolock

Simple Autolock is available on *MERCURY-VX*, *MERCURY*, and UNITY*INOVA*, UNITY*plus*, or *GEMINI 2000* as a software function and on UNITY and VXR-S as a hardware function:

- Software simple Autolock searches for the correct Z0 value in software, but does not adjust lock power, gain, or phase.
- Hardware simple Autolock searches for the lock resonance over an approximately 10 ppm range, turning up the lock power by 3 dB from its preset value during the search and then turning the lock power back down when lock has been found and captured.

Once energized, this type of lock remains energized until simple Autolock is selected again or optimizing autolock is selected.

A danger in hardware simple Autolock is that if the lock signal falls below a certain level, the system reenters the lock capture phase and boosts the lock power. This can have unfortunate consequences during, for example, a shimming operation.

Using the Acquisition Window

Applies only to UNITY and VXR-S systems configured for acquisition.

1. If the Acquisition window is not open, enter `acqi` in the input window, then click on the Connect button in the window when it appears.
2. Click on the LOCK button.

   The LOCK display appears. The LOCK menu near the top of the display has three choices: off, on, and auto.
3. Click on auto.

Using the Input Window

Applies only to all systems but type of Autolock (software or hardware, see above) depends on the system.

- Enter `alock='y'`

  Autolock is activated at the start of acquisition if it has not already been activated.

Optimizing Autolock

Optimizing Autolock uses a sophisticated software algorithm to search the field over the full range of Z0 (as opposed to hardware simple Autolock), captures lock, and automatically adjusts lock power and gain (but not lock phase).

Using the Input Window

- Enter `alock='a'` or `alock='s'`.

  If `alock='a'`, at the beginning of each experiment (each initiation of an acquisition), the system searches for the lock signal if necessary, and then optimizes lock power and gain (but not phase) whenever an acquisition is initiated with `go`, `ga`, `au` or with any macro or menu button using the `go`, `ga`, or `au`.

  If `alock='s'`, the same process as `alock='a'` occurs but only if the sample has just been changed under computer control and `go`, `ga`, or `au` is entered (when manually ejecting or inserting a sample, the software cannot keep track of the action and `alock='s'` has no effect).

If `z0` is inactive and you start an autolock operation with either the `lock` command or by setting the `alock` parameter to an appropriate value, then `autolock` searches for the lock signal by changing the lock frequency. Figure 36 is an example of a lock frequency acquisition window.

Be aware that spectrometer frequencies are computed from the lock frequency, so if the lock frequency changes as a result of an Autolock operation, frequencies for that acquisition will be off by the amount of that change. Switching from chloroform to acetone requires a change in the lock frequency of about 5 ppm, which can cause problems in precision work. Changing lock frequency is only a problem when you select Autolock with

the `alock` parameter. It is *not* a problem for the lock experiment, since, by definition, the lock experiment is complete once the autolock operation is completed.

Using GLIDE

1. If the *GLIDE* interactive window is not open, enter `glide` in the input window or click on the GLIDE button in the Main Menu.
2. Click on the Setup icon.
3. Choose an experiment and solvent.
4. Click on the Setup button.
5. Click on the Custom icon.
6. Click on the Acquire icon.
7. In the Locking field, click on Auto.

   Z0, lock power, and lock gain are optimized.

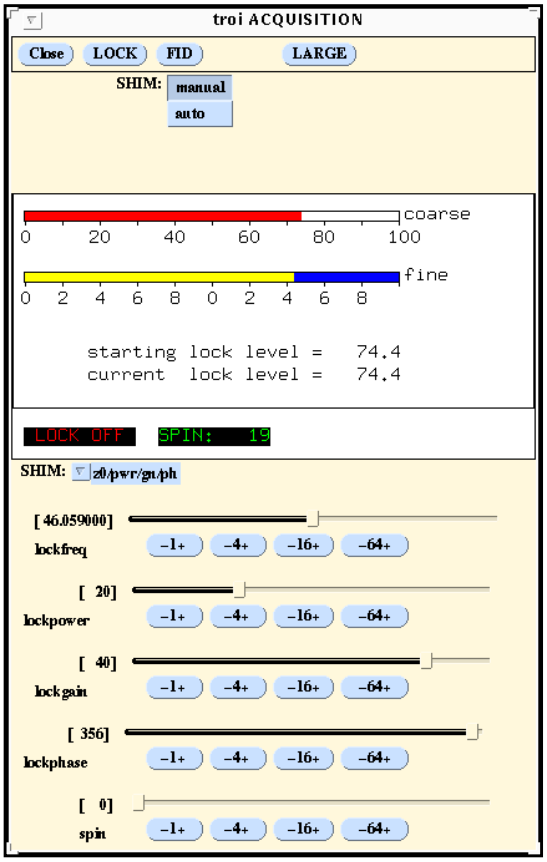


Figure 36. Lock Frequency Acquisition Window

Full Optimization

Full optimization is the most complete optimization of lock parameters. A fuzzy logic auto-lock algorithm automates the parameter control process in order to find the exact resonance and the optimum parameters (phase, power, gain) automatically and quickly with high reliability. Fuzzy rules are used in the program to find the exact resonance frequency and for adjusting power and phase. The fuzzy rules are implemented at different stages of the auto-lock process. First, the software finds the resonance. If the exact resonance cannot be found, phase and power are adjusted and the software looks for the exact resonance again. The software then optimizes the lock power to avoid saturation, optimizes the lock phase, and optimizes the lock gain to about half-range.

RF frequencies, decoupler status, and temperature are also set during full optimization.

Using the Input Window

- Enter `lock`

  Note that the full optimization is the *only* automated method for optimizing the lock phase. If `alock='a'` or `'s'` is entered, only power and gain is optimized.

Lock Level and Spin Speed Error Handling

The `in` parameter controls error handling based on lock level and spin speed, and specifies the action to be taken based on lock level failure or spinner failure:

- `'n'` stops any system checking so that acquisition continues regardless of the lock channel or spin speed.
- `'w'` makes the system check the lock level and the spin speed. A warning message is added to the log file if the lock level falls below a preset hardware level (about 20 on the lock meter) or if the `spin` parameter is set to a particular value and the spin speed goes out of regulation; however, acquisition is not stopped.
- `'y'` makes the system check the lock level and spin speed. Acquisition is halted if the lock level falls below a preset hardware level (about 20 on the lock meter) or if `spin` is set to a particular value and the spin speed goes out of regulation.

The `in` parameter can be set to one or two characters:

- If set to two characters, the first character specifies the action for lock failure and the second character specifies the action for spinner failure.
- If set to only one character, that character specifies the same action for either lock or spinner failure.

Lock Loop Time Constant Control

During acquisition, the `lockacqtc` parameter sets the *lock loop time constant*, the time constant by which the lock feedback corrects disturbances of the magnetic field. On a UNITY*INOVA* or UNITY*plus*, `lockacqtc` is `1`, `2`, `3`, or `4`, which corresponds to time constants of 1.2, 4.7, 12, or 48 seconds, respectively. On a UNITY or VXR-S, `lockacqtc` is `1` or `2`, for 1 or 200 seconds. *MERCURY-VX*, *MERCURY*, and *GEMINI 2000* do not use `lockacqtc`.

When the system is not performing an acquisition (idle, lock display, shim display, FID display, autoshim, etc.), the `locktc` parameter (not available on *MERCURY-VX*, *MERCURY* and *GEMINI 2000*) controls the lock time constant. The values for `locktc` are the same as for `lockacqtc`.

These parameters do not normally exist in the software. The system uses the slowest value for `lockacqtc` (`4` for UNITY*INOVA* or UNITY*plus*, and `2` for UNITY or VXR-S) and the fastest value (`1` on all systems) for `locktc` if the parameters do not exist. To try other values, you can create one of the parameters and give it a value by entering, for example, `create('lockacqtc','integer','global')` `setlimit('lockacqtc',4,1,1,'global') lockacqtc=1.` You do not need to create both parameters.

6.9 Adjusting Shims

Shim coils are small magnetic fields used to cancel out errors in the static field. In shimming, the current to the shim coils is adjusted to make the magnetic field as homogeneous as possible. Computer-controlled digital-to-analog converters (DACs) regulate the room-temperature shim coil currents. Every time a new sample is introduced into the magnet or probe is changed, it is necessary to readjust the shims.

Shim Gradients

The shims are actually printed coils wrapped round a cylindrical form that encloses the NMR probe. A coil (or sum of coils) whose field is aligned along the axis of the magnet is called a Z axial shim gradient (Z1, Z2, Z3, etc.). Coils whose fields are aligned along the

other two orthogonal axes are called X and Y radial shim gradients (X1, XY, X2Y2, Y1, YZ, etc.). The field offset coil Z0 ("zee-zero") alters the total magnetic field.

Each shim gradient is controlled by its own parameter; for example, the X1 shim gradient is controlled by a parameter named `x1`. For Z1 and Z2 gradients there are two parameters for each: `z1` and `z2`, which are the "fine" gradients, and `z1c` and `z2c`, which are the "coarse" gradients. In addition, the field offset is controlled by a parameter `z0`. The full set of shim gradient parameters is displayed by entering `dgs`, which causes the group of shim parameters to be displayed.

Depending on the value of the `shimset` parameter, shim values range from –2047 to +2047 or from –32767 to +32767, with a value of zero producing no current. The limits for each shim gradient are listed in the *VNMR Command and Parameter Reference*.

The macro `readallshims` reads all shims from the hardware and sets the values into the shim parameters in the current parameter tree. The shims used depend on the `shimset` configuration. For the shim set on the Ultra•nmr shim system, `readallshims` is active only if hardware-to-software shim communication is enabled. `readallshims` is not available on *GEMINI 2000* systems.

The macro `setallshims` sets shims from the current parameter tree into hardware. `setallshims` is equivalent to entering `load ='y'su` but without setting all the hardware parameters normally set by `su` (temperature, decoupling, transmitter initialization, etc.). The shims used depend on the `shimset` configuration. For the shim set on the Ultra•nmr shim system, `setallshims` is active only if hardware-to-software shim communication is enabled. `setallshims` is not available on *GEMINI 2000*.

Methods of Shimming

Depending on the system, homogeneity adjustments can be made on the spectrometer by a number of manual and automatic methods:

- Direct keyboard entry
- Retrieving previous shim values
- Manual emulation mode
- Interactive autoshim
- Background autoshim
- Fully automatic autoshim
- Hardware Z1 autoshim
- Gradient autoshim

Each method is described below. Table 16 lists the commands and parameters described for shimming. For a general discussion about shimming, refer to the manual *System Administration*.

Shimming using the Ultra•nmr shims system is covered separately in "Shimming Using the Ultra•nmr Shim System" on page 164.

Keyboard Entry

Shim values can be entered "by hand." Such parameter changes are active or not active according to the setting of the `load` parameter.

Table 16. Homogeneity Adjustment Commands and Parameters

Commands	
`acqi*`	Open the Acquisition window
`dgs`	Display shim & automation parameter group
`diffshims(shimfile1,shimfile2)`	Compare two sets of shims (VNMR)
`diffshims shimfile1 shimfile2`	Compare two sets of shims (UNIX)
`dshim<(file)>,dshim('method'|'help')`	Display a shim "method" string
`gmapshim<('files'|'mapname'|'quit')>`	Start gradient autoshimming
`newshm`	Interactively create shim method
`readhw(par1,par2,…)<:var1,var2,…>`	Read acquisition hardware values
`rts(file)<:status>`	Retrieve shim coil settings
`sethw*`	Set acquisition hardware values (shim-related)
`shim`	Submit an Autoshim experiment
`stdshm`	Interactively create a shim method
`svs(file)<:status>`	Save shim coil settings
`* acqi<('par'|'disconnect'|'exit'|'standby')><:ret>`	
`* sethw(<'wait'|'nowait',>par1,val1<,par2,val2,...)`	
Parameters	
`gmap_findtof {'n','y'}`	Find tof before start of gradient shimming.
`gmap_z1z4 {'n','y'}`	Gradient shim z1-z4, then higher-order shims.
`hdwshim {'n','y','p'}`	Hardware shimming (if available)
`hdwshimlist {'z1','z1z2x1y1'...}`	List of shims for hardware shimming
`load {'n','y'}`	Load status of displayed shims
`method {file in shimmethods}`	Autoshim method
`shimset {1,2,3,...14}`	Type of shim set
`shimspath {absolute path}`	Path to user's shims directory
`wshim {'n','e','s','g','f','f#'}`	Conditions when to shim
`x1, y1, z1,...`	Shim gradients X1, Y1, Z1, ...
`z0 {-2048 to 2047, –32768 to 32767}`	Z0 field position

Using the Input Window

1. For each of the shim values you want to change, enter the shim gradient parameter with the new value (e.g., `z1=247`).
2. To load the new values, enter `load='y' su.`

Saving and Retrieving Shim Values

Previous shim values can be retrieved and used in the current experiment. For routine operation on undemanding samples (for example, polymers with broad lines), this may be completely sufficient. The different computer-controlled shim gradients are always set to the values at the end of the last shimming operation; therefore, it is never *necessary* to retrieve old shim values when starting a new sample.

If it is possible to assume that the previous sample was run by a reasonably skilled operator on a sample comparable to the current one, shimming can be resumed where it was terminated on the previous sample. This mode is selected by setting the parameter `load='n'`, meaning do not load new shim values. If, on the other hand, the state of the shims is unknown, it may be preferable to start by resetting the shims to known values. This is done by retrieving a set of shim values, or by entering values as desired, and then setting `load='y'`, followed by `su`.

Shim settings can be stored to reflect different combinations of probe, solvent, sample height, nucleus or magnetic environment. At a minimum, a shim set should be saved for each solvent name: `cdcl3`, `acetone`, etc.

Using the Input Window to Save Shim Coil Settings

- Enter `svs(file)`, where `file` is the name of a file for saving shim coil settings (e.g., `svs('acetone')`).

  If `file` is an absolute path, `svs` uses it to save the file. Otherwise, it saves the file in the user's `shims` directory. If that directory does not exist, it saves it to directory named by the `shimspath` parameter. If `shimspath` does not exist, it saves the file in the system `shims` directory (provided the proper permission mode is set).

  The macro `diffshims(shimfile1,shimfile2)` compares the values for the room-temperature shims stored in two separate files written using `svs`.

Using the Input Window to Retrieve Saved Shim Coil Settings

1. Enter `rts(file)`, where `file` is the name of a file containing shim coil settings to be retrieved (e.g., `rts('acetone')`).

   If `file` is an absolute path, `rts` uses it to find the file to retrieve. Otherwise, it checks for the file in the user's `shims` directory. If that directory does not exist, it checks for the file in the directory named by the `shimspath` parameter. If `shimspath` does not exist, it retrieves the file in the system `shims` directory. After the file is retrieved, `rts` sets `load='y'` to facilitate loading of the shims.

   The `rts` command also extracts the shim parameter values from a parameter or data sets saved with macros `svf` or `svp` and sets `load='y'` to facilitate subsequent loading of shims. (The commands `su`, `shim`, `go`, `ga`, and `au` reset `load='n'` to prevent a subsequent inadvertent loading of the shims.) Thus, if a sample is to be rerun on the same probe and under the same conditions for which an earlier experiment has already been performed and stored, settings for the repeat run can be initialized by retrieving the shim values from the earlier run.

   When a shim set is retrieved, whether from a `shims` directory or from a data set, only the shim parameter values have been changed. The actual shim currents are only altered if `load='y'` and `su`, `shim`, `go`, `ga`, or `au` is entered. If `load='n'`, each of these programs begins with the actual shim currents and not those specified by the parameters in the current experiment. Also, if `load='y'`, the Acquisition window does not return shims.

2. Execute the `listenon` macro.
3. Activate CDE.
4. Start the file manager from the tool bar and go to the directory that contains the file you want to retrieve.
5. Use the mouse to double-click on the file name.

Manual Emulation Shimming

The most familiar method of homogeneity adjustment to many users is the manual emulation mode, which is accessed with the Acquisition window. For the procedures in using this mode, see "FID/Spectrum Shimming Windows" on page 154.

In this mode, the mouse is used to interactively select and display different combinations of four or five shim controls that can be used to manually adjust the homogeneity while

observing a lock level, real-time FID display, or real-time spectrum display on the screen. For small amounts of “touch-up” shimming, this method may prove to be the fastest (short of simply retrieving old values); however, it is certainly not the most reliable in an open access environment with users of differing skill levels, nor is it applicable to fully automated operation using a sample changer.

Automated Shimming

Like locking, shimming can be done manually as already described. Automated shimming is often preferred, however. It can be initiated the following ways:

- *Interactive Autoshim* – Opening the Acquisition window and clicking on the auto button in the SHIM display (described on page 143).
- *Background Autoshim* – Entering `method=file shim` (e.g., if the file is `z1z2`, enter `method='z1z2' shim)` in the input window (described on page 145). This method is analogous to using the `lock` command for full optimization of lock parameters.
- *Fully automatic Autoshim* – Setting the parameter `wshim` (analogous to `alock`) at the beginning of an acquisition or series of acquisitions (described on page 144).
- *Hardware Autoshim* – Setting the parameter `hdwshim` (described on page 145). Available only on UNITY*INOVA* systems or UNITY and VXR-S systems with the Z1 shimming hardware. This method is analogous to hardware simple Autolock.

No matter how the automated shimming is initiated (except hardware Z1 Autoshim), it is controlled by two aspects of the shimming process (each aspect is discussed in detail in subsequence sections):

- *Quality or criterion for shimming* – The quality of the field homogeneity when the automated shimming is started must be given and the quality of the homogeneity at the conclusion of the shimming must be specified.
- *Method used to shim* – For routine “tweaking” of the resolution, adjustment of Z1 and Z2 is sufficient, and the method `'z1z2'` would be selected. In the interactive Autoshim mode, this is one of six methods accessible by pull-down menu after auto is selected. A variety of standard shim methods are available in the `vnmr/shimmethods` library. You can use the `dshim` macro to display the available shim methods. You can also create your own shim method and store it in your user `shimmethods` (for `vnmr1`, the path would be `/export/home/vnmr1/vnmrsys/shimmethods` on Solaris, or `~vnmr1/vnmrsys/shimmethods`.

  If you decide on a particular method for routine work, it would be wise to save it in the standard parameter set for each nucleus to which it is applicable.

Automatic shimming relies on a non-saturating lock signal on which an optimizing process can be performed. If too high a lock power is used, the shimming process can become unreliable since it may be chasing a “moving target.” Since it is customary to increase lock power until the lock level maximizes, if done manually, it is clear that lock signals will be partially saturated. This follows directly from the shape of a saturation curve where signal amplitude increases linearly with lock power until a point where it flattens out, becomes oscillatory, and eventually declines.

Adjustment for maximum lock level puts the lock power near the top of this curve. The response of the lock level to changes in gradients is not as sensitive as in a non-saturating case, and therefore automatic shimming is not as reliable. Nonsaturating lock power is easily checked by determining if the lock level changes by the proper factor of two upon a change of 6 dB in lock power. Usually, acetone-d_6 must have at least 8 to 15 dB less power than $CDCl_3$, for example, to remain non-saturated.

Shimming Criteria for Autoshim

In all forms of automatic shimming, whether interactive or noninteractive, another concept, the shimming criterion, enters into the process. Two aspects of Autoshim must in some way be specified by the user. One is the resolution of the starting point—good or bad? If good, only small changes need to be made to the shim settings to find the optimum; if bad, larger changes are necessary. The second is how good must the final resolution be? Clearly, the better the desired resolution, the smaller the steps that Autoshim must take as it approaches the maximum in order to find the absolute maximum to within a specified degree.

As shown in Table 17, for each there are five criterion values: B (bad), L (loose), M (medium), T (tight), and E (excellent). (The lower-case letters are used when entering criterion values into a shim method, discussed below.)

Table 17. Permissible Shimming Criterion Values

Criterion	*Meaning*	*Recommended Usage*
B or b	Bad	No decent starting shim values available
L or l	Loose	Extreme change in sample height
M or m	Medium	Typical sample change
T or t	Tight	Resolution desired above average
E or e	Excellent	Resolution desired less than 0.2 Hz

A full criterion consists of two letters, for example, L > M indicates a loose starting criterion (the shims are expected to be far from their desired values) and a medium ending criterion (end with “normal” shim quality). Tight and excellent are only used for extremely high resolution where the beginning resolution is very nearly that desired.

Thus, if you suspect that the resolution is poor and want to improve it rapidly but not spend the time necessary to get excellent resolution, you might specify the starting and ending points as L >M. In the interactive Autoshim mode, these criteria are specified on a pull-down menu after clicking the auto button in the SHIM display.

The time of automatic shimming is a function of these criteria. Therefore, try to make an informed choice in light of the resolution needed and, in particular, for FID shimming, the choice of acquisition time `at` specified in the parameter table. An acquisition time of 2 seconds gives a limiting *digital* resolution of 0.5 Hz, a resolution that would be inconsistent with shimming to a tight criterion. In the interactive shimming mode using `acqi`, only the most important criteria are accessible to the user: L > M, M > M, M > T, and T > T (B and E are inaccessible).

The starting criterion should never affect the final result, only the time in which that result is produced. If the starting criterion is specified as T, for example, and the optimum shim is far off, this shim will eventually be found. The search will, however, take longer than if a starting criterion of L had been specified.

Shim Methods for Autoshim

A shim method consists of a text string contained in a file within the VNMR system’s or a user’s `shimmethods` directory. That text string will be interpreted as a series of instructions describing the shimming method. Commands in elements include:

- Turn on and off the spinner
- Set maximum shim time per element

- Set the delay between lock level samplings
- Specify the gradients to be shimmed and the criterion used for shimming.

A complete method consists of one or more elements, separated by commas and terminated with a semicolon (e.g., `f,ry,t600,szq:cmm;`). The element setting which specific gradient or gradients to be shimmed has the syntax `sxx:cyz`, where `s` identifies the shim part of the form, `xx` is a two-character code for a specific shim gradient or gradient combination, `c` identifies the criterion part of the form, `y` is the starting criterion, and `z` is the desired ending criterion.

Table 18 lists standard two-character codes for shim gradient combinations.

Table 18. Codes for Standard Shim Gradient Combinations

Standard Code	*Gradients*	*Hexadecimal Code*
`z1`	Z1C	`0000008`
`z2`	Z2C	`0000020`
`z3`	Z3	`0000040`
`z4`	Z4	`0000080`
`z5`	Z5	`0000100`
`zq`	Z1C, Z2C	`0000028`
`zt`	Z1C, Z2, Z3	`0000068`
`zb`	Z1C, Z2C, Z4	`00000A8`
`za`	Z1C, Z2C, Z3, Z4, Z5	`00001E8`
`ze`	Z2C, Z4	`00000A0`
`zo`	Z1C, Z3, Z5	`0000148`
`zc`	Z1C, Z2C, Z5	`0000128`
`zm`	User-selected gradients	User-entered
`tx`	X, Z1	`0010004`
`ty`	Y, Z1	`0020004`
`t1`	X, Y, Z1	`0030004`
`t2`	X, Y, XY, YZ, X2Y2, Z1	`03B0004`
`tz`	X, Y, XZ, YZ, Z1	`0270004`
`tt`	X, Y, XZ, XY, X2Y2, YZ, Z1	`03F0004`
`t3`	X, Y, XZ2, YZ2, Z1	`5030004`
`t4`	X, XZ, X3, XZ2, Z1	`4450004`
`t5`	Y, YZ, Y3, YZ2, Z1	`1A20004`
`t6`	XY, X2Y2, ZX2Y2, ZXY, Z1	`A180004`
`t7`	X, Y, XZ, XY, X2Y2, YZ, X3, Y3, YZ2, ZX2Y2, XZ2, ZXY, Z1	`FFF0004`
`ta`	X, Y, XZ, XY, X2Y2, YZ, YZ2, XZ2, Z1	`53F0004`
`tm`	User-selected gradients	User-entered

Refer to the description of the `shimset` parameter in the *VNMR Command and Parameter Reference* for a list of shims in each type of shim set.

The following examples show the meaning of a few standard shim methods:

- `szq:cmm;` means set shims Z1C and Z2C with a medium to medium criterion.

- `sza:clm;` means shim all Z gradients with a loose to medium criterion.
- `szt:clm,szb:clm,szq:cmm;` means shim Z1C, Z2, and Z3 with a loose to medium criterion, then shim Z1C, Z2C, and Z4 with a loose to medium criterion, and lastly shim Z1C and Z2C with a medium to medium criterion.

User-Defined Shim Methods for Autoshim

The shim methods supplied with the system are based on a series of "standard" coil groupings; however, you may wish to perform an automatic shimming operation using other groups of shims than are provided. For example, you might wish to shim Z1, Z3, and Z4 while holding Z2 fixed.

To allow this operation, certain combinations of shims coils can be selected by constructing a 7-digit hexadecimal (base 16) number based on the shim coil diagram in Table 19.

To construct a method for this example, first notice in the diagram that Z1 is represented by a 4 in the first digit (on the far right) and that Z4 and Z3 are represented by a 8 and 4, respectively, in the second digit, which gives a total of 12 (or C in hexadecimal notation). The rest of the digits are 0 because no other shimming is desired. Thus, the seven-digit hexadecimal number representing Z1, Z3, and Z4 is `00000C4`. This number is then prefixed by *zm* or *tm* (the two are equivalent) making `szm00000C4` the method desired.

Some examples of user-selected methods:

- `stm0A30004:clm;` means shim Z1, X1, Y1, YZ, Y3 with loose to medium criterion.
- `szm0000108:cmm;` means shim Z1C and Z5 with medium to medium criterion.

To make it easier to modify the standard shim gradient combinations, the hexadecimal code for each standard coil grouping is listed in the third column of Table 18.

The following codes enable control of other aspects of automatic shimming:

- `l` sets shimming on the lock instead of the FID (default).
- `f` sets shimming on the FID instead of the lock (background FID shimming is not available on *MERCURY-VX*, *MERCURY*, and *GEMINI 2000* systems).
- `f:0,90` sets shimming on the FID with limits for the FID evaluation range. Full range is 0 to 100 percent of the duration of the FID. Sensitivity to higher-order spinning gradients is increased with a start of 0 and a finish limit of about 5 or 10, which weights the evaluation to the front of the FID.
- `ry` (rotation yes) turns the spinner on.
- `rn` (rotation no) turns the spinner off.
- `dx` sets a delay *x* hundredths of seconds between lock samplings. Variations in lock solvent T_1 and T_2^* relaxation times affect the ability of automatic shimming to attain good resolution in reasonable times. If too short, automatic shimming will not perform properly. If too long, the shimming will become unacceptable in duration. `dx` allows setting an appropriate delay and can be used one or more times within a text string. If no entry is made using `dx`, the system automatically measures the lock response and sets a delay accordingly.
- `tx` sets the maximum shimming time to *x* seconds. Once `tx` is set, it governs all future shim elements within a method string, just as `dx` governs the lock sampling interval for all shim elements until changed. If `tx` is not set, the shimming will proceed based on internal program criteria.

Table 19. Hexadecimal Codes for Shim Groups

8 4 2 1	8 4 2 1	8 4 2 1	8 4 2 1	8 4 2 1	8 4 2 1	8 4 2 1
ZXY XZ2 ZX2Y2 YZ2	Y3 X3 YZ X2Y2	XY XZ Y1 X1	— — — —	— — — Z5	Z4 Z3 Z2C Z2	Z1C Z1 Z0 —

- `q` recalls an algorithm's internal parameters so that shimming starts quickly. `q` is a background autoshim that keeps the magnetic field at an optimum during experiments of long duration. Shimming is performed at the time `wshim` instructs. Only the portion of the shim methods following the letter `q` is executed after the experiment's first increment. Any shim method may follow `q`; however, the `sz1` (Z1 only) and `szq` (Z1, Z2) are the most effective. Multiple shim methods may follow `q`, but time effectiveness is reduced.

Methods may be entered into the `shimmethods` file using a text editor such as `vi`. The macros `newshm` and `stdshm` provide an interactive method of defining shim methods. Note that unlike normal text files, which have unrestricted size, the maximum text file size for a shim method is 128 characters.

The following examples show complete user-defined shim methods:

- `szq:cmm,rn,stz:cmm,ry,szq:cmm;` means shim Z1C, Z2C with medium to medium criterion, turn off spinner, shim X, Y, XZ, YZ, Z1 with medium to medium criterion, turn on spinner, and then shim Z1C, Z2C again with medium to medium criterion throughout.
- `d50,szq:cmm,d150,sza:cmm;` means to sample every 0.5 seconds while shimming Z1C, Z2C, and then to sample every 1.5 seconds while shimming all Z gradients. Use medium to medium criterion throughout.
- `t60,szq:cmm,t240,sza:cmm;` means shim Z1C, Z2C for 60 seconds maximum, then shim all Z gradients for a maximum of 4 minutes. Use medium to medium criterion throughout.
- `f,ry,t600,szq:cmm;` means turn on spinner and FID shim Z1C, Z2C with medium to medium criterion for 10 minutes maximum (not available on *GEMINI 2000*).
- `t60,sza:cmm,q,t30,sz1:cmm;` (with `wshim='f20'`) means initially shim on all Z gradients for 60 seconds, then shim Z1. After every 20 FIDs, shim Z1 for 30 seconds.
- `sza:cmm,q,t30,szq:cmm;`(with `wshim='f10'`) means initially shim on all Z gradients (with no time out) and then perform a Z1, Z2 shim for 60 seconds every 10 FIDs.

Interactive Autoshim

To enter the interactive Autoshim mode, from the Acquisition window, do the following:

1. Open the SHIM display
2. Use the mouse to make a series of choices for computer shimming, perhaps the Z1 and Z2 gradients, and select a criterion, such as L > M.
3. Click on the auto button in the SHIM display to initiate Autoshim.

After completion of that shim operation, you can select a different combination of gradients and begin another autoshim process, or you can terminate the entire process at that point. For further information, refer to “SHIM Display” on page 161.

If desired, interactive Autoshim and manual emulation modes can also be interspersed. The interactive Autoshim mode is particularly useful to give the user a feel for the operation of Autoshim and the relative importance of the different gradients under different conditions such as different size samples or different sample heights.

Fully Automatic Autoshim

In the fully automatic Autoshim mode, the parameter `wshim` controls the automatic shimming activity. `wshim` can specify no shimming, shimming at the start of data acquisition, etc. Shimming in each case is initiated by some form of data acquisition, whether by a command `go`, `ga`, `au`, or a macro using one of these commands.

Using the Input Window

- For shims on the lock signal, set `wshim` to `'n'`, `'e'`, `'g'`, or `'s'`, where:
  `'n'` indicates no automatic shimming is performed. Even with `wshim` set to this value, the shimming procedure specified by the parameter `method` can be activated by using the `shim` command.
  `'e'` indicates automatic shimming is done for the experiment prior to data acquisition.
  `'g'` indicates that automatic shimming *using gradient shimming* is done only at the beginning of the first experiment, following the change of sample using the automatic sample changer. The parameter `method` is ignored. This value is available only in automation and is not used with the `go`, `ga`, or `au` commands. See “Gradient Autoshimming” on page 168 on how to set up gradient shimming before using this method.
  `'s'` indicates automatic shimming is done only at the beginning of the first experiment, following the change of a sample using the automatic sample changer.
- For shims on the FID, enter `'f'` or `'f`*n*`'` (*n* is an integer), where:
  `'f'` indicates automatic shimming is done prior to the data collection of each new array member in a multi-FID experiment (not available on *MERCURY-VX*, *MERCURY*, and *GEMINI 2000*).
  `'f`*n*`'`, where *n* is an integer, indicates shimming is done prior to data collection of every nth FID. For example, `wshim='f16'` will shim prior to acquiring FIDs 1, 17, 33, etc. This method is only relevant to arrayed or 2D experiments (not implemented on *MERCURY-VX*, *MERCURY*, and *GEMINI 2000*).

Using GLIDE

1. If the *GLIDE* interactive window is not open, open it entering **`glide`** in the input window or by clicking on the **GLIDE** button in the Main Menu.
2. Click on **Setup**.
3. Choose an experiment and solvent.
4. In the AutoSHIM field, click on **YES**.
5. Click on **Setup** > **Custom** > **Acquire**.
6. Click on **Do** > **Close**

Background Autoshim

Background Autoshim is controlled by the parameter `method` and the command `shim`. This is a complete background Autoshim method that provides no interaction with the operator whatsoever. The type of automatic shimming to be done during routine sample changes depends on the level of homogeneity required on any particular sample, the change in sample height, and the maximum time desired for shimming.

- For average homogeneity needs with samples which are either long or all of identical height, simple `z1z2` shimming is usually sufficient.
- If sample height might vary, the method `allzs` has been found to be the most reliable, at the expense of greater time spent in shimming. This method shims first Z1, Z2, and Z4, then Z1, Z2, and Z3, and finally Z1 and Z2.

The standard parameter sets `stdpar/h1` and `stdpar/c13` have `method` set to `z1z2`. If you find that more shimming is routinely necessary in your applications, simply recall those parameter sets, change `method` to `allzs` (or another method of your own devising) and save the parameter set, overwriting the original parameter set.

Using the Input Window

- Enter **`method=`*`file`* `shim`**, where *`file`* is the name of a file in the directory `shimmethods` (e.g., `method='z1z2' shim`).

  Two `shimmethods` directories can exist. A user can have a private copy of `shimmethods` in a personal `shimmethods` directory. A system-wide set of shim methods is also located in the `/vnmr/shimmethods` directory. The user's private library is searched first for a given method. If the method is not found in the user's directory, then the directory `/vnmr/shimmethods` is searched.

  Shimming methods can be used in succession or strung together. For example, entering `method='lz12m' shim shim` would cause the method in the file `lz12m` (Z1, Z2 shimming) to be used, as indicated by its code, twice in succession, and entering `method='lz12m' shim method='nsm' shim shim shim` would cause the first method to be used once and the second method three times.

Hardware Autoshim

Hardware autoshim methods vary according to which system is involved.

UNITY *INOVA Systems*

The `hdwshim` parameter enables the commands `go`, `ga`, or `au` to turn on and off hardware autoshimming, which is done using a software emulation of hardware autoshim. Shimming is active only while a pulse sequence is executing:

- If `hdwshim='y'`, shimming is active only during the first delay of the pulse sequence.
- If `hdwshim='p'`, shimming is active only during the first presaturation pulse, defined as a change in power level followed by a pulse (e.g. `presat.c`).

Shimming during subsequent delays or presaturation pulses can be activated by using the `hdwshiminit()` statement before the delay or presaturation pulse. Shimming uses the `z1` shim by default.

If the parameter `hdwshimlist` is created, shimming uses the specified list of shims to shim on. Only the following shims are allowed:

`z1`, `z1c`, `z2`, `z2c`, `x1`, `y1`

Shimming is done in the order of `z1`, `z1c`, `z2`, `z2c`, `x1`, `y1`, regardless of the order in which the shims are used in `hdwshimlist`, and is performed on each shim in intervals of 20 seconds. The fine shims (`z1`, `z2`, `x1`, and `y1`) are recommended for routine use.

UNITY and VXR-S Systems with Z1 Shimming Hardware

The `hdwshim` parameter enables commands `go`, `su`, `au`, etc. to turn on and off the Z1 shimming hardware. Hardware shimming is automatically suspended during software autoshimming.

MERCURY, UNITY*plus*, and *GEMINI 2000* Systems

Hardware autoshimming is not available.

Using the Input Window

- Enter **`hdwshim='y' su`**
  On UNITY*INOVA*, hardware shimming starts at the next acquisition during the first delay, and stops when acquisition is complete.
  On UNITY and VXR-S, this command turns on hardware Z1 shimming.
- Enter **`hdwshim='p' su`**.
  On UNITY*INOVA*, hardware shimming starts at the next acquisition during the first presaturation pulse, and stops when acquisition is complete.
  On UNITY and VXR-S, this command does not activate shimming.
- To turn off shimming, enter **`hdwshim='n' su`**.

Gradient Autoshim

First, confirm that gradient shimming is installed on your system and that the shims are mapped with gradient shimming. If the gradient shimming is not installed, see “Gradient Autoshimming” on page 168.

Gradient autoshimming can be initiated by any of the following ways:

- Using the Menu Buttons

  In the Main Menu, click on **Setup** > **Shim** > **Gradient Autoshim on Z**. Current parameters and data are saved, and gradient shimming is started in the current experiment. Parameters and data are retrieved when gradient shimming is finished.

  To stop gradient shimming before shimming is completed, in the Main Menu, click on **Setup** > **Shim** > **Quit Gradient Shim.** Quitting aborts the experiment and retrieves the previous parameter set and data. This button does not appear if gradient shimming is not running.

- Using the Input Window

  To start gradient shimming, enter `gmapshim`. This is the same as clicking on **Gradient Autoshim on Z**.

  To stop gradient shimming before it completes, enter **`gmapshim('quit')`**. This is the same as clicking on **Quit Gradient Shim**.

- Automation

  Use **`wshim='g'`** within automation parameter sets (applies only to UNITY*INOVA*, UNITY*plus*, *MERCURY-VX*, or *MERCURY* systems). See “Fully Automatic Autoshim” page 144, or the `wshim` entry in the *VNMR Command and Parameter Reference*.

Which Shims to Use on a Routine Basis

The following suggestions should assist you in routine shimming, especially on shim systems with a larger number of shim channels:

- *Establish and maintain lineshape* – Use Z to Z5, possibly Z6, X, Y, ZX, ZY, and possibly Z2X and Z2Y. The effects of Z7 and Z8 (and realistically Z6) are too small to see with the lineshape sample.
- *Shim a new lineshape sample of different geometry* – Use Z to Z5, possibly Z6, X, Y, ZX, ZY, and possibly Z2X and Z2Y.
- *Shim a new sample of the same geometry* – Use Z, Z2, and maybe Z3.
- *Shim a new sample of different geometry* – Use Z to Z4 and possibly Z5, X, Y, ZX, ZY.
- *Shim for water suppression* – Start with a shim set that produces a good lineshape for the same sample geometry. Next, tweak Z and Z2, and then vary Z5 and Z7 to minimize the width of the base of the water (Z and Z2 may need to be tweaked if Z5 changes by more than 100 to 200 coarse units). About 80 to 90 percent of the odd-order axial-gradient induced water width is probably dominated by Z5, with Z7 and perhaps some Z3 providing the rest.

  The even-order axial shims (Z2, Z4, Z6, and Z8) affect the asymmetry of the residual water line (using presaturation). All four of these even-order axial shims can affect the final water linewidth, with Z2 and Z4 being at about the 5 mM solute level and above, Z6 being at about the 1 mM solute level, and Z8 being at about the 0.3 mM solute level. The even-order axial shims will perform as you would expect unless the sample is less than 40 mm in length, in which case the shims still control the water linewidth but much less responsively.

  Beware of the use of Z4 to narrow an asymmetric residual water line of a sample shorter than about 40 mm. One is probably destroying the base of the standard lineshape faster than the residual water signal is being narrowed. This is because the residual water resonance width is affected more by magnetic susceptibility interfaces as the sample gets shorter. For samples under 40 mm, the iterative use of Z5-Z7 with Z6-Z8-Z4-Z2 can narrow the residual water line, but the results obtained may be hard to reproduce on subsequent samples due to an increased sensitivity to slight changes in sample geometry.

Shimming Different Sample Geometries

Some suggestions when moving the sample:

- *Moving the same sample up* – Z, Z3, and Z5 need to become more positive.
- *Shortening and centering (moving up) the sample* – Z2 and Z4 need to become much more positive. The trends for Z and Z3 are mixed and more complex, but they tend to become a little more negative. It appears as if Z and Z3 are driven positive as the sample is pulled up, but they are driven negative faster as the sample shortens. When shimming a lineshape sample, plan on the following changes (starting from lineshape shims for a 700 µL sample at a depth 67-68 mm):

  700 µL to 600 µL: move Z2 +50 DAC units and move Z4 +250 units.
  700 µL to 500 µL: move Z2 +200 units and Z4 +600 units.

  The Z2 and Z4 changes track well with sample volume, but are relatively independent of tube depth. It is therefore easiest when changing sample geometries to make the appropriate Z2 and Z4 corrections, then adjust the more complex Z1-Z3-Z5 interactions as needed.

6.10 Using the Acquisition Window

The Acquisition window, also called the interactive acquisition window or `acqi` window, provides many capabilities, including:

- Turning sample spinning on and off.
- Adjusting lock.
- Selecting manual or automatic shimming, and adjusting shim values if manual shimming is selected.
- Displaying the FID or spectra in real time.
- Changing parameter values interactively (not available on *MERCURY-VX*, *MERCURY* and *GEMINI 2000* systems).
- Controlling the eject air to insert and eject the sample (only if the spin control hardware is present).

Table 20 lists the commands and parameters associated with this window.

Table 20. Interactive Acquisition Commands and Parameters

Commands	
`acqi<:$ret>`	Open the Acquisition window
`acqi('par')`	Send selected parameters to `acqi`
`acqi('disconnect')`	Disconnect from `acqi` program
`acqi('exit')`	Exit `acqi` program
`acqi('standby')`	Start `acqi` program and put in standby mode
`gf`	Set parameters for FID/spectrum display
`go*`	Submit experiment to acquisition
`su`	Submit a setup experiment to acquisition
`* go<(<'acqi'><,'nocheck'><,'nosafe'><,'next'><,'sync'><,'wait'>)>`	
Parameters	
`dmgf {'av'}`	Absolute-value display of FID data or spectrum in `acqi`
`phfid {–360 to 360 deg,'n'}`	Zero-order phasing constant for the `np` FID

Opening the Window

The Acqi button is automatically available in the Main Menu when VNMR is started. Otherwise, to open an Acquisition window, enter the `acqi` command in the input window.

To successfully use the `acqi` command, your system must be configured for acquisition; you cannot use `acqi` on a data station. Entering `acqi` on a data station causes the message "`Cannot run acqi, acquisition communication not active.`"

In macros, `acqi` can be given a return value to determine its success or failure of running.

Acqi Button

Under normal circumstances on a spectrometer, when you start VNMR, an Acqi button appears in the Main Menu.

However, this button does not appear if VNMR is immediately started after an installation, before the system is configured, if a user's `bootup` macro has been changed to keep `acqi` from starting, or on systems configured as data stations. If you do not see the Acqi button,

and your system has been configured as a spectrometer, enter `acqi('standby')` to display the button.

Entering `acqi` without arguments on a command line starts the `acqi` program and (if no acquisition is in progress) displays an Acquisition window, shown in Figure 37.

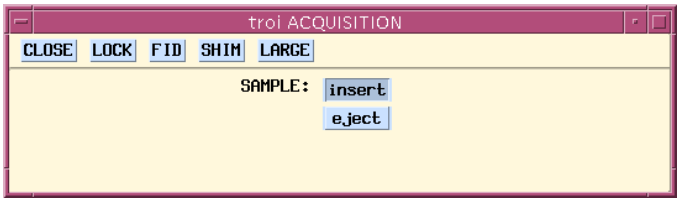


Figure 37. Acquisition Window (`acqi` Program)

Note: The "disconnected" Acquisition window, which initially appeared after the command `acqi` was entered, no longer exists. It has been replaced by the Acqi button in the Main Menu.

On all systems except UNITY*INOVA*, if you start an acquisition and then click on the Acqi button, the window does not appear.

On UNITY*INOVA* systems, if you start an acquisition and then click on the Acqi button, an abbreviated selection of buttons, similar to Figure 38, appears.

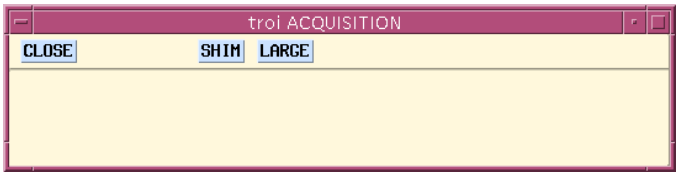


Figure 38. Abbreviated Acquisition Window

On all systems, when `acqi` has already been started by another user, you will be unable to open the Acquisition window by clicking on the Acqi button.

If `acqi` is successfully started, the Acqi button in the Main Menu vanishes.

There is now a CLOSE button in each Acquisition window. Clicking this button causes the `acqi` window to disappear and the Acqi button to reappear in the permanent VNMR menu panel.

Connecting to the Acquisition System

After you click the Acqi button or enter the `acqi` command, the Acquisition window, shown in Figure 37, is displayed on the right side of the main VNMR display. The initial window has five buttons that are selected by clicking with the left mouse button:

CLOSE	Causes the Acqi button in the Permanent VNMR menu to reappear. The VNMR command `acqi('disconnect')` is equivalent to clicking the CLOSE button. If `go` or `su` is typed in the input window, `acqi` disconnects and returns the parameters, and then the command is started within VNMR.
LOCK	Opens the LOCK display (described on page 151).
FID	Opens the FID display (described on page 154). From the FID display, you can select the Spectrum display (described on page 159)
SHIM	Opens the SHIM display (described on page 161).
LARGE	Generates a larger graphics window. This might be useful to you, for example, when shimming on larger magnets or when tuning the probe and you need to observe the screen. To return to the standard size graphics window, click the SMALL button (notice that the SMALL button appears in place of the LARGE button when the LARGE button is selected).

If the spin control hardware is installed, the Acquisition window also contains the SAMPLE menu with the following choices:

insert	Turns off the eject air, waits for the sample to slowly drop, then turns off the slow drop air. After sample is seated, all buttons are displayed again.
eject	Turns on the eject air and slow drop air to eject the sample from the probe. At this point, most buttons disappear, and a sample *must* be inserted (or at the least the insert button selected) before continuing.

Making a Choice in a Display

As you make choices in the LOCK, FID, Spectrum, and SHIM displays, the contents of the window change and the indicated actions take place.

To make a choice in a display, the quickest way in most cases is to move the mouse cursor arrow on top of the choice you want, then click once with the left mouse button.

To see the range of choices for a menu:

1. Move the mouse cursor arrow to the menu button.
2. Click on the *left* mouse button to cycle through all possible choices.

To use a pop-up menu instead of a regular menu:

1. Move the mouse cursor arrow to the menu button.
2. Hold down the *right* mouse button. A pop-up menu appears with a menu of the choices available.
3. Continue to hold down the right mouse button. As the mouse cursor arrow is dragged up or down the menu, each selection in turn is highlighted. When the choice you desire is highlighted, release the right button. Your choice is selected and the pop-up menu disappears.

Changing Parameter Values

If changes are made to lock, shim, gain, and spin parameters in the LOCK, FID, Spectrum, and SHIM displays, the new values are returned to VNMR only by clicking the CLOSE button. If the current experiment has the parameter `load` set to `'y'`, the shim values are not returned to that experiment.

However, if changes in `lockpower` and `lockgain` are made in VNMR (e.g., entering `lockpower=lockpower-10`), the Acquisition window does not learn of the change if it is disconnected but not exited. To get the new values in to the Acquisition window, you must type `su` or and click on the Acqi button to restart.

If changes to `lockpower` and `lockgain` are made only within Acquisition window, there is no problem. When the Connect button is clicked, the `acqi` program reads all shims and lock parameters from the acquisition computer, so that entering `lockpower=10 su`, then clicking the Connect button sets `lockpower` to 10 within `acqi`. This is independent of the `load` parameter.

When changes to a display are made in rapid succession (especially in FID when long delays are used), the mouse may seem inoperative. This becomes apparent when the left mouse button no longer inverts the panel buttons or when the right button brings up the Frame menu instead of inverting the Panel button. When this happens, wait for the next update of the graphics window, then proceed.

LOCK Display

The LOCK display appears when the LOCK button is clicked from any Acquisition window. Figure 39 shows a typical LOCK display.

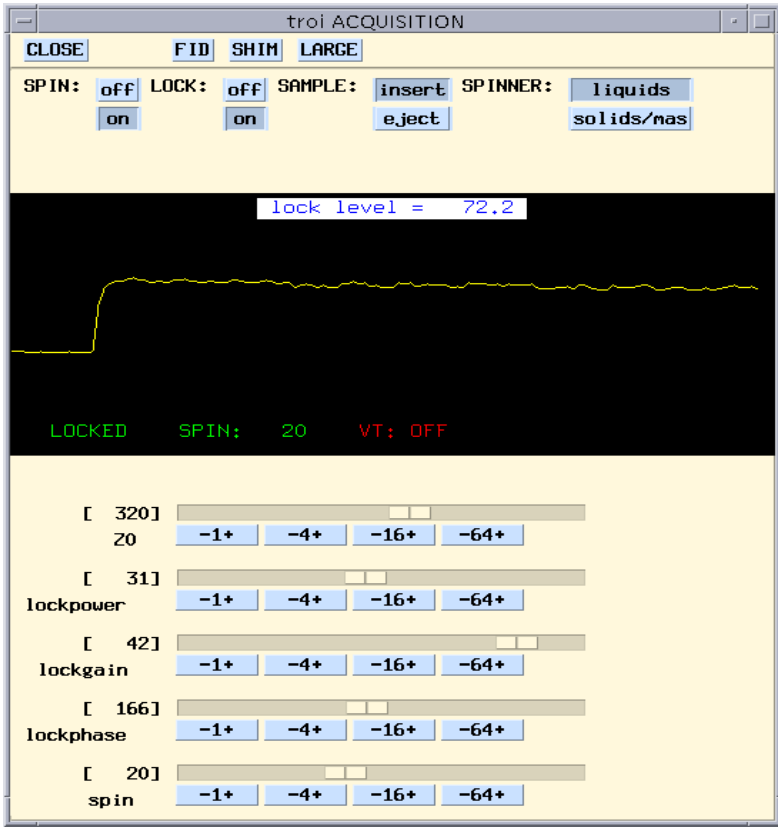


Figure 39. LOCK Display Window (`acqi` Program)

At the top of the LOCK display is a row of buttons labeled CLOSE, FID, SHIM, and LARGE—these buttons were described above. Below these buttons are the SPIN, LOCK, and (optionally) SAMPLE menus:

- SPIN sets sample spinning off and on.
- LOCK sets lock to off, on, or auto (auto is available only on UNITY and VXR-S systems). Selecting auto chooses hardware simple Autolock, which is described on page 132.
- SAMPLE controls inserting and ejecting samples if spin control hardware is installed. This menu was described above.

The central part of the window shows the lock signal and, below that, the current status for lock, spin, and the variable temperature (VT status is displayed only if the `vttype` parameter is not 0). Color is used to identify status conditions:

- LOCKED is displayed in green if locked, NOT LOCKED in yellow if not regulated, and LOCK OFF in red if lock is off.
- SPIN: # (where # is the current spin rate, for example, SPIN: 15) is displayed in green if spinning is regulated (within 1 Hz from the requested value), SPIN # in yellow if not regulated, and SPIN: OFF in red if the spinner is off.

- VT: # (where # is the current temperature in °C) is displayed in green if VT is regulated (temperature is within 0.5 °C from the requested value), VT: # in yellow if the temperature is not regulated, and VT: OFF in red if VT is off.

The lower section of the LOCK display window contains controls for changing the values of the lock parameters `z0`, `lockpower`, `lockgain`, `lockphase`, and `spin` (optional on *MERCURY* and *GEMINI 2000*). The current value of each parameter is displayed as a number and as a slide control (a horizontal bar with the slide at a position proportional to the value of the parameter). The value of the parameter controlled by the slide control can be altered by dragging the mouse cursor across the slide control with the left button of the mouse held down.

If z0 is inactive, then `acqi` shows a `lockfreq` slider/button array instead of showing a z0 slider/button array. The range is ±2000 Hz. Buttons are labelled in Hz, and allow the lock frequency to be modified in increments of 1 Hz, 4 Hz, 16 Hz, and 64 Hz. Find the lock in exactly the same manner as you would finding lock using z0. However, on UNITY*INOVA*, the granularity of resolution for lock frequency is approximately 2.3 Hz, so changes in the lock frequency of 1Hz or even 2 Hz might not change the frequency sent to the lock circuit in the probe.

Alternatively, the value of each parameter can be changed by clicking on the four buttons marked –1+, –4+, –16+, and –64+ (on the *GEMINI 2000*, `lockgain` only has a –10+ button and it can only be set to 0, 10, 20, or 30). Each click with the *left* mouse button on one of these buttons *subtracts* the value shown; each click with the *right* mouse button *adds* the value shown. For example, to add 14 to the parameter `lockpower`, move the mouse cursor arrow to the–16+ button in the row for lockpower and click the right mouse button once. Next, move the arrow to the –1+ button in the same row and click the left button twice.

Using lockfreq to Find Lock Resonance

In VNMR 6.1 and *only* on UNITY*INOVA*, you can find the lock signal or resonance by using either the `z0` parameter or the lock frequency. If you use the lock frequency, then less shimming when switching solvents and less adjustment to the lock phase should be required.

To choose `z0`, you must activate `z0`; to choose lock frequency, you must deactivate `z0`. If `z0` is inactive, then the system uses the lock frequency to find the lock signal. If `z0` is active, the system uses `z0`.

To activate `z0`, enter `z0='y'`; to deactivate `z0`, enter `z0='n'`.

lkof Parameter

On UNITY*INOVA* systems only, a new global parameter, `lkof`, has been added to track changes in the lock frequency resulting from changes in the solvent, and minor changes caused by the magnet drifting. The current lock frequency is the sum of the system global parameter `lockfreq` and `lkof`. The units for `lockfreq` remain MHz. The units for `lkof` are Hz; analogous to `sfrq` and `tof`, or `dfrq` and `dof`. `lkof` affects two components of the system: autolock on the console and `acqi` on the host computer.

When either `acqi` disconnects or an experiment completes, VNMR changes `lkof` to reflect the new lock frequency in the console, if `z0` is inactive.

Using sethw to Set Lock Frequency

On only UNITY*INOVA* and *MERCURY-VX* and *MERCURY* systems, the lock frequency can be set with the `sethw` command. To set the lock hardware, type the following command:

```
sethw('lockfreq', <lockfreq value>)
```

The units for the lock frequency are in megahertz.

Be aware that `go`, `lock`, `shim`, `su`, and related commands reset the lock frequency in the console to the current value of the lockfreq parameter. On UNITY*INOVA* systems only, this value is offset by the value of `lkof`, if that parameter exists.

Simple Locking

Establishing lock using simple or manual locking uses the LOCK display. The line that crosses the spectral window represents how close the deuterium resonance field is to the lock frequency. When the two are matched, the line should be flat (with perhaps some noise, depending on the lock gain and lock power). The poorer the match, the greater the number of sine waves in the line. Figure 40 represents the changes from a bad match to a good match.

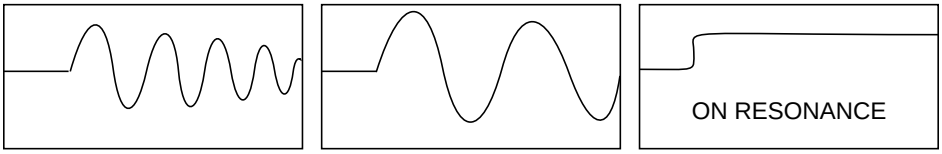


Figure 40. Finding Lock

The following procedure for finding lock manually is typical:

1. Make sure a sample is inserted and seated properly. Spinning helps but is not required.
2. In the LOCK menu at the top of the window, click the off button.
3. Using the slide control, –1+, –4+, –16+, and –64+ buttons, or entering values directly, turn up lockpower and lockgain, and look for some sinusoidal variation in the signal.

   The actual value needed for lockpower and lockgain depends upon the concentration of the deuterated solvent, the nature of the deuterated solvent—the number of deuterium atoms per molecule—and the relaxation time of the deuterium. At this point, do not be too concerned about optimizing power and gain; just look for a sine wave.
4. If you see no sine wave (perhaps just noise), click on the –16+ button for Z0 until some discernible wave appears.
5. If you know the concentration of the lock solvent is high, say greater than 50%, turn down the lock power.

   If the lock power is too high, the deuterium nuclei become “saturated,” the signal oscillates (goes down and then back up), and it is difficult to establish lock. The correct amount of lock power is difficult to determine, but it is helpful to remember that acetone is more easily saturated than most solvents.

6. Adjust Z0 until the signal changes from a sine wave to an essentially flat line. If the solvent is concentrated, the line may start to move up on the screen as the lock condition is approached.

7. In the LOCK menu, click the on button.

   The signal should move up and look like the on-resonance diagram in Figure 40. If the lock signal displays a dip at the point where it starts or the signal slopes downward, incorrect lock phase is the probable cause. To adjust phase, use the SHIM display because it is much easier to use the thermometer-like indicator on this display for phase adjustment. Select z0/pwr/gn/ph from the SHIM menu in the SHIM display.

FID/Spectrum Shimming Windows

The FID/Spectrum display appears first when the FID button is clicked from any Acquisition window. VNMR provides two styles of FID shimming. The Style 1 FID shimming window is shown in Figure 41 and the Style 2 FID shimming windows are shown in Figure 42. Clicking on the Style 1 or Style 2 button near the top of the display toggles between the two styles.

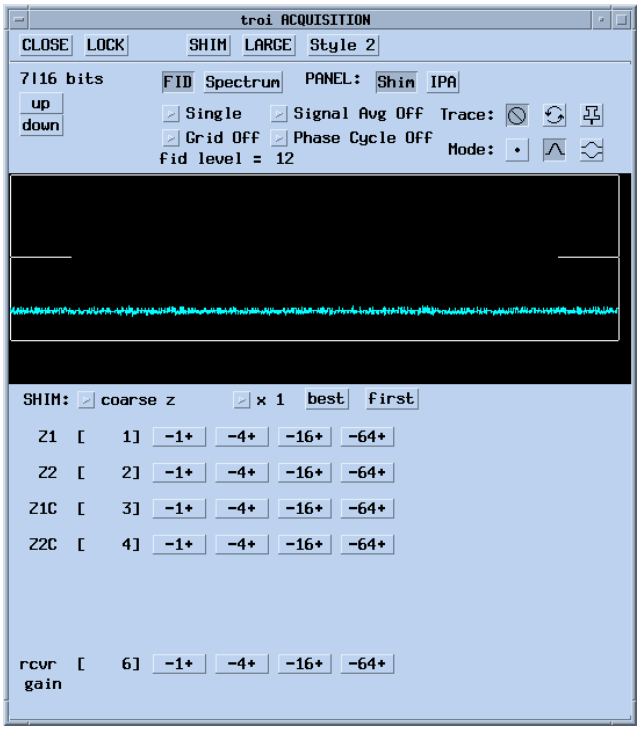


Figure 41. Opening Style 1 FID/Spectrum Display Window (`acqi` Program)

Style 2 FID shimming is not available on VXR-S or UNITY systems that have an output board with a 63-step FIFO. It is also not available on *GEMINI 2000*, *MERCURY*, or *MERCURY-VX* systems.

Before selecting the FID/Spectrum display, an experiment must be set up within VNMR. Any experiment type can be used. In an arrayed or multidimensional experiment, the first element is used. Entering the macro `gf` then submits the experiment for display by the `acqi` program but does not initiate data acquisition from the experiment. Using `gf` prevents certain acquisition events from occurring, such as spin control and temperature change.

The command `go('acqi')` can be used instead of `gf` but is not recommended. In using `gf` to control the acquisition of data, the parameters `alock` and `wshim` are disabled, `load` is set to `'n'`. The value of `nt` is not relevant; the experiment continues indefinitely until you leave the FID/spectrum display. The current values of `lockpower`, `lockgain`, and `lockphase` parameters within `acqi` are used. Autogain (`gain='n'`) can be used, but it slows down the appearance of the first FID.

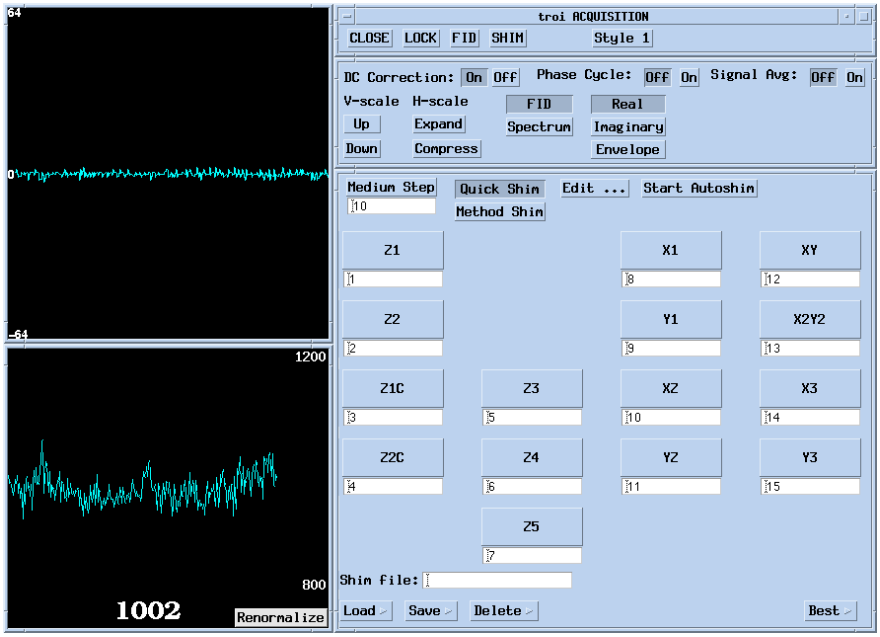


Figure 42. Style 2 FID Shimming Display in Real-time (`acqi` Program)

FID Shimming Window (Style 1)

Figure 41 shows a typical Style 1 FID/Spectrum display. In the opening FID/Spectrum display, the FID is observed in a graphics window at the center of the display.

At the top of a FID display are a row of buttons—CLOSE, LOCK, SHIM, and LARGE. These buttons were described on page 149.

Below these buttons, on the left, are buttons labeled up and down. These buttons adjust the number of bits of the ADC that are displayed; for example, 14|16 bits means 14 bits of a 16-bit ADC make full scale on the display.

Near the center is a menu with choices FID and Spectrum. The label of the currently active display is highlighted. Selecting Spectrum in this menu changes the FID/Spectrum display to display the spectrum for the FID (described on page 159).

To the right of the SMALL/LARGE button is the style button that allows you to switch between Style 1 and Style 2 FID shimming. Shimming on the FID is discussed on page 160.

Below this menu are two toggle buttons (shown as Single and Grid Off in Figure 41). (On the INOVA system, there might be two more buttons, see the following subsection “Style 1 Interface.”). The currently selected choice is displayed. The toggle button on the top left alternates between the choices Single and Summed:

- Single button displays the last acquired FID. A yellow box indicates the ADC limits, and two short yellow lines indicate the zero point of the ADC. If the display is down scaled, the ADC limit is indicated by short red lines in the display.
- Summed button displays the summed FID.

The toggle button on the below left alternates between Grid and Grid Off. Clicking on this with the left mouse button toggles the display of grid lines overlaying the FID display. The grid lines are provided as an aid to monitoring the effects of changing the shims.

Style 1 Interface

On UNITY*INOVA* systems, on the right of the Single/Summed and Grid switches are two more toggle switches—the Signal Avg switch to the right of the Single/Summed switch, and the Phase Cycle switch to the right of the Grid switch.

When the Signal Avg switch is turned on, the pulse sequence runs blocksize (`bs`) transients before returning data to the interactive program. When Signal Avg is turned off, it runs one transient. To change the number of Signal Avg transients, change the `bs` parameter and run `gf` to update the acodes.

When the Phase Cycle switch is turned on, the default phase cycling will be turned on (`cp='y'`) and will cycle the phase over `bs` transients even if Signal Avg is off. When the Phase Cycle is off, the default phase cycling will be turned off (`cp='n'`).

Further to the right are labels for Trace and Mode, which control the display of the FID in the window. Trace has these choices:

- Clicking on the slashed circle sets the trace to off, the default.
- Clicking on the recycle symbol shows the current trace (in blue) and the previous trace (in yellow) so the traces can be compared.
- Clicking on the pin makes current FID stay the same color (in blue) and updates the previous FID (in yellow). To select a new current FID, click on the pin again.

Mode has the following choices:

- Clicking on the dot puts the FID display into a dot mode, mostly useful for solid-state NMR. The dot display mode only works if it can be displayed; that is, the value of `np` is small enough so the data points can be separated.
- Clicking on the single curve sets the standard FID display mode, the default.
- Clicking on the double curves sets an envelope display that shows the outline of the FID envelope.

The FID display is controlled by the acquisition parameters active when the `gf` or `go('acqi')` command is executed and by the processing parameters `lsfid`, `phfid`, and, if present, `dmgf`. The `gf` macro is recommended instead of running `go('acqi')` directly. Using `gf` prevents certain acquisition events from occurring, such as spin control and temperature change. Changes to acquisition parameters become active in the Acquisition window after the execution of `gf` or `go('acqi')`. Changes to the three processing parameters become active in `acqi` after the execution of `acqi('par')`.

The lower panel of the FID display window contains menus and buttons for changing the shim parameters:

- SHIM menu selects the group of shim parameters (up to six) to be manually adjusted (e.g., the axial z menu is shown in Figure 41).
- x1 button toggles the magnitude of the shims adjustment buttons. Selecting x32 changes the increments from –1+ –4+ –16+ –64+ to –32+ –128+ –512+ –2048+.
- best button reloads shims that gave the best lock level in the current session (valid only if the `lockgain`, `lockpower`, and `lockphase` parameters are unaltered).
- first button reloads shims to the values that existed at the start of the current session.

Below the SHIM menu are the shims controls. Each shim can be adjusted between minimum and maximum values by the buttons to the right of the value. Clicking a button with the *right* mouse button *adds* the value shown on the button; clicking with the *left* mouse button *subtracts* the value shown on the button.

Generally there are one, two, or three panels of Z (spinning) shims, between two and five panels of non-spinning shims, and one panel of lock parameters. Each of the shims should be adjusted to give maximum homogeneity and “spin” (top area of window) and lock parameters adjusted appropriately.

The bottom row of buttons adjust the lock receiver gain. Note that when in the FID display window these buttons adjust the observe receiver gain.

The macro `gf` provides a convenient way to set up an interactive acquisition session. `gf` temporarily disables autogain, spin regulation, and receiver phase alternation, sets `wshim='n'` and `alock='n'`, and then runs `acqi('par')` and `go('acqi')`. Note that if the Acquisition window closes when the FID button is closed, it is usually because no `gf` or `go('acqi')` was executed.

Typical actions in using `acqi` for a FID display are the following:

1. Make sure you have good parameters by acquiring a spectrum with `ga`.
2. When is spectrum is acceptable, enter `gf`.
3. Click on the Connect button followed by the FID button.

FID Shimming Windows (Style 2)

Style 2 FID shimming is not available on VXR-S or UNITY systems that have an output board with a 63-step FIFO. It is also not available on *GEMINI 2000* or *MERCURY* systems.

Style 2 provides shimming on either the FID or the Spectrum. Figure 42 shows FID shimming selected.

The Style 2 shim button area is arranged to accommodate the number of shims in the installed shim set. Selecting a shim button with the left mouse button decreases the shim value by the amount shown on the Fine Step/Coarse Step button. Clicking on the button with the right mouse button increases the value by the same amount, while clicking on it with the middle mouse button toggles the Fine Step/Coarse Step between fine and coarse. The sizes of the coarse and fine steps are selected by clicking the left or right mouse button on the Fine Step/Coarse Step button. Other ranges besides coarse and fine can be created by editing the file `$HOME/.acqirc`. Shim values can also be typed directly into the fields where they are displayed—you need to press Return to download the entered value.

Select a shim to be included in Quick Shim by holding the shift key down while clicking any of the three mouse buttons on the desired shim button. Doing the same action a second time deselects the button. The buttons thus selected are displayed highlighted. The shims selected this way are optimized when Quick Shim is active and the Start Autoshim button is clicked.

Autoshimming with a predefined method is also possible. First, a method must have been created and saved, as described in “Editing Autoshim Methods” below. Then select Method Shim, select a method from the menu, and click Start Autoshim.

The buttons at the bottom left of the control panel allow you to load, save and delete shim values in named files. Click the left mouse button to load, save, or delete the named file, or click the right button to select a file name from the menu. The Best button at the bottom right resets the shim values to the best seen in the current session when clicked with the left mouse button. (The Best button may not give correct results if the DC Correction status has been changed. Select Reset Best from the menu to reset the record of best shim values.)

The main display screen shows the FID or spectrum in real time, depending on what has been selected on the control panel. On UNITY*plus* and older systems, the displayed data is signal-averaged over `nt` transients.

Style 2 Interface

On UNITY*INOVA* systems, there are two toggle switches, Phase Cycle and Signal Avg, next to the DC Correction switch. As in the Style 1 interface, they allow you to phase cycle and/or signal average the data over bs transients.

The vertical scale is controlled by the Up and Down buttons and the horizontal scale by the Expand and Compress buttons. Each click of one of these buttons changes the scale by a factor of two.

The Real, Imaginary, and Envelope choice buttons allow you to view either channel alone, or the square root of the sum of the squares of both channels.

The history of the quality of the shimming, as measured by the area under the FID envelope, is displayed by the Quality Meter, shown in Figure 42.

The shim quality is calculated from the area in the FID envelope. The large number at the bottom is the latest value of the shim quality, arbitrarily scaled to a reasonable range. Clicking the Renormalize button resets the scaling factor such that the next value displayed is 1000. The vertical scale of the graph is automatically adjusted to keep the most recent value in view.

Editing Autoshim Methods

Clicking the Edit button on the Style 2 shim control panel displays the Autoshim Method Editor, shown in Figure 43.

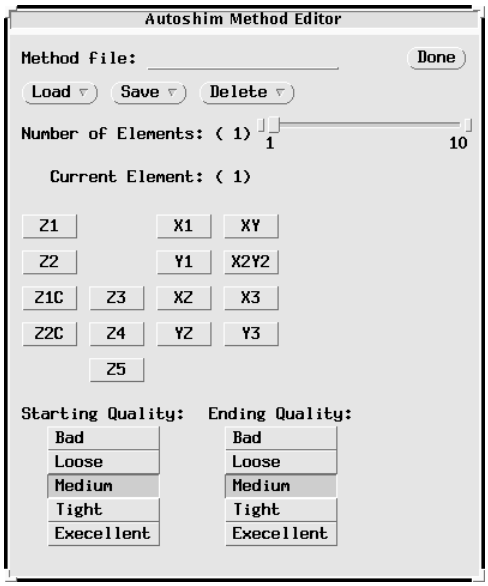


Figure 43. Autoshim Method Editor Panel (`acqi` Program)

An autoshim *method* consists of a series of autoshim *elements*. Each element of the method optimizes the values of a selected group of shims. The elements are executed in order to obtain the final shim values. The number of elements in the user's method is selected in the Elements field. The user edits one element at a time; the Current Element field selects which one is currently being changed.

Within a particular element, the user selects which shim coils to optimize by selecting the desired shim buttons with the left mouse button. (A selected coil can be deselected by selecting it again with the mouse.) The buttons at the bottom of the window allow the user to specify an estimate of the starting shim quality and a specification of how tight to make the convergence criterion.

The buttons at the upper left of the window allow the user to load, save, and delete shim methods. A method must be saved before it can be used.

Spectrum Display

Figure 44 shows the FID/Spectrum display window with a typical spectrum display (Style1). The spectrum display can also be viewed in Style 2. The menus and buttons in the window are the same as for the FID display except that vertical scaling is represented as a multiplier, shown near the top left corner (e.g., x4 means the data is multiplied by 4). Multipliers available include x1, x2, x4, x8, x16, and x32. The up and down buttons select the vertical scaling multiplier.

The spectrum display is controlled by the additional parameters `sp`, `wp`, `dmg`, `rp`, `lp`, `rfl`, `rfp`, `vs`, `vp`, `sw`, and `fn`. The same limits on the acquisition parameters as those described for the FID display apply to the spectrum display. Furthermore, if the Fourier number parameter `fn` is greater than 64K, it is reduced to 64K.

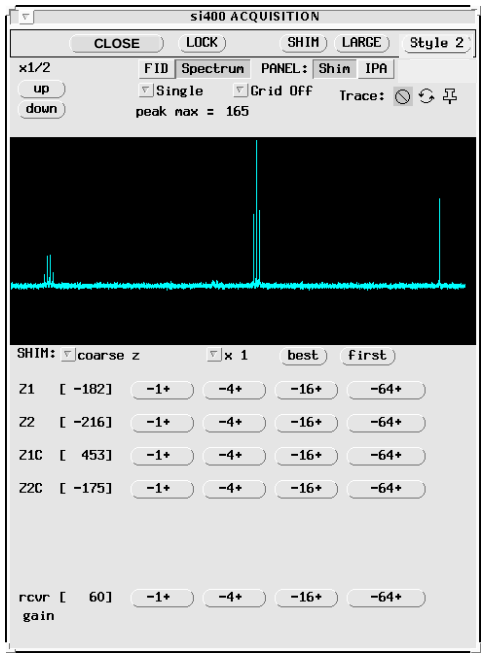


Figure 44. Spectrum in FID/Spectrum Display Window (`acqi` Program)

These parameters are automatically sent to `acqi` when `acqi` is first invoked. They can subsequently be changed and sent again to `acqi` with `gf` or `acqi('par')`. This is exactly analogous to the way the FID parameters are sent to `acqi`.

Interactive Parameter Adjustment

In interactive parameter adjustment (IPA, not available on *MERCURY-VX*, *MERCURY*, and *GEMINI 2000*), if the pulse sequence used for `go('acqi')` or `gf` contains statements such as `ipulse` or `idelay`, or if the parameter `phfid` is not set to NOT USED, a menu labeled PANEL appears to the right of the FID/Spectrum menu with the following choices:

- Shim selects the shim adjust button in the bottom panel to enable you to adjust the displayed shims while observing the FID. To select different shims to adjust, select a different choice from the SHIM menu. At the bottom of the display are buttons for adjusting the shims or parameters. To increase a shim or parameter value, click with the right mouse button on the button with the value you want to increase; to decrease a value, click with the left mouse button instead. Adjustment of shims and parameters was discussed previously in this chapter.
- IPA selects interactive parameter adjustment in which the bottom panel displays up to five slide control and button combinations. Figure 45 shows IPA selected with slide controls and button combinations for the parameter `phfid` on display.

  Each slide control and button combination has a menu button on the left (showing only the current selected value), which serves as a label to identify which parameter is adjusted. By clicking the right mouse button on this label, a menu appears showing the parameters that can be adjusted by the current pulse sequence. You can select any one of the parameters shown and the slide control and button combination will adjust the newly selected parameter. This way, when more than five parameters need to be adjusted, any combination of five can be selected to show in the bottom window. The

value of the parameter is displayed in a square bracket, such as `[10.0]`, to the right of the menu button.

If the pulse sequence is written with multiple `ipulse` statements, for example, and the same label is provided to the different `ipulse` statements, a single slide control is present and changing the value of that slide control affects all pulses simultaneously. For further information on IPA statements, see *VNMR User Programming*.

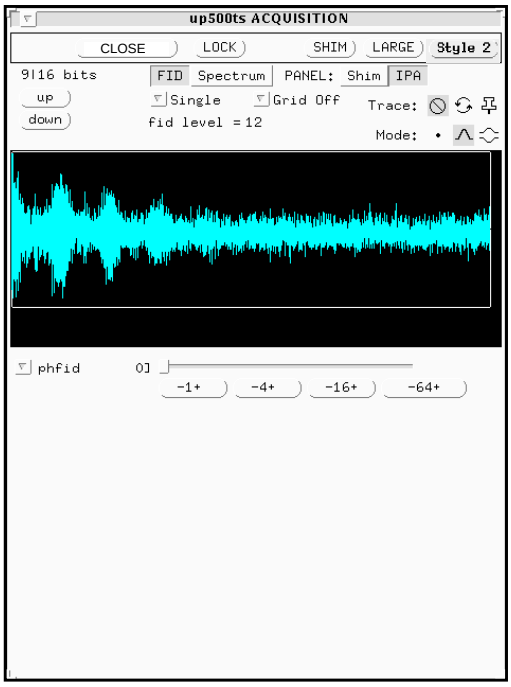


Figure 45. Spectrum Display Window with IPA (`acqi` Program)

Shimming on the FID

The strategy for shimming on the FID is somewhat different from that of shimming on the lock. In general, the adjustments are made on the basis of the shape of the FID, not on its amplitude. The best single criterion is that one is attempting to increase the signal strength of the FID across the FID display.

Best results can be initially obtained by selecting parameters so that, with `nt` set to `1` and the `d1+at` at approximately 1.0, an off-resonance FID with good signal-to- noise at the beginning and pure noise at the end is observed in the `df` display. This may require adjustment of `pw`. Once this is obtained, enter `gf` and go to the interactive FID display. Select Style 1 or Style 2 FID shimming.

Shimming on the Spectrum

As most shimming is done in order to obtain a “correct” spectrum, the strategy for shimming on the spectrum is somewhat obvious. For a first time, it is recommended that a well-shimmed sample with a singlet be used. You can then make an intentional misadjustment in a shim and observe the effect on the spectrum.

A suggested procedure for shimming is the following:

1. Set `phfid=0`.
2. Enter `go` to acquire a spectrum. Process it and expand the display to focus on the peak(s) of interest.
3. Enter `gf`.
4. In the Acquisition window, click on Connect | FID | Spectrum
5. If the spectrum is not at the correct vertical intensity, adjust the vertical scale multiplier with the up and down buttons.
6. If a phase correction is required, click on IPA in the PANEL menu, then adjust phfid as an alternative to rp, hence phasing the spectrum.

7. Click on Shim in the PANEL menu, then shim in the normal way, using the lineshape of the peaks as a shimming criterion.
8. If the sample is not locked, adjust `z0` to shift the spectrum.
9. If you wish to make changes to the display (such as altering `sp`/`wp`), make the changes in VNMR by entering the command `ds` to display the spectrum and altering the required parameters.

   When you have a satisfactory display, enter `gf` or `acqi('par')` to send the changes to the Acquisition window. Then click on LOCK | FID. The next display should reflect the changes.

SHIM Display

The SHIM display appears when the SHIM button is clicked from any Acquisition window. Figure 46 shows a typical SHIM display. The buttons at the top of the window (CLOSE, LOCK, FID, LARGE) and the menus and buttons in the lower panel (SHIM, x1, best, shim adjustment, first, lockgain) were described previously.

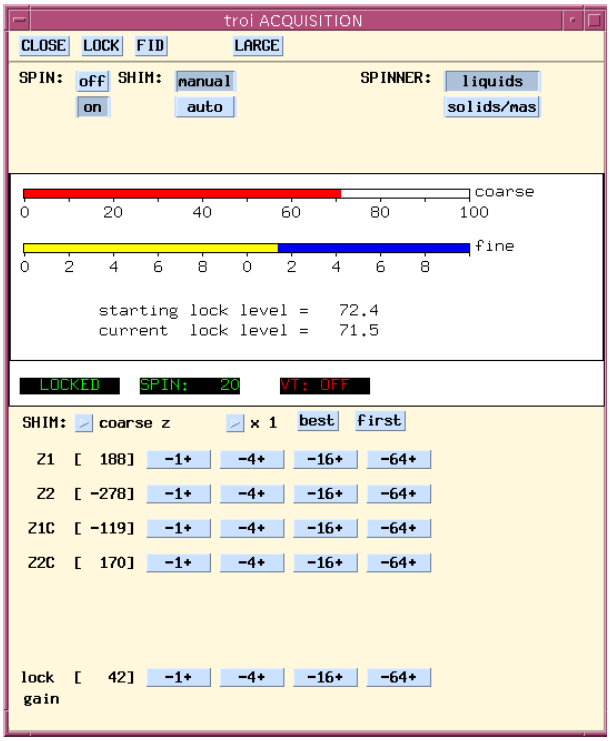


Figure 46. SHIM Display Window (`acqi` Program)

In the upper panel are the SPIN and SHIM menus:

- SPIN sets sample spinning on or off. This menu was described in the section covering the LOCK display.
- SHIM sets the mode of shimming: manual mode performs manual shimming, and auto mode performs automatic shimming. Each is described next.

Manual Mode

In the manual mode, up to six shims can be displayed for adjustment. Using the SHIM menu to select sets of shims and adjusting shim values is covered in “FID/Spectrum Shimming Windows” on page 154.

Auto Mode

In the auto mode, the bottom of the window changes to one button and two menus (shown in Figure 47):

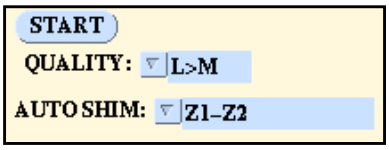


Figure 47. Auto Mode Window (`acqi` Program)

- START button starts the shimming process. When shimming starts, the button label changes to STOP. Clicking on STOP will stop the shimming.
- QUALITY menu selects the shimming criteria—loose (L), medium (M), or tight (T)—and the order used (for example, L > M means start with loose shimming and end with medium shimming). The selection is made with the mouse in the normal way. Refer to "Shimming Criteria for Autoshim" on page 140 for more information.
- AUTOSHIM menu holds the selections of shim combinations that can be adjusted. Choices on this menu include Z1-Z2, Z1-Z4, and ALL NONSPINS. A selection is made with the mouse in the normal way, the criteria set, then shimming is started. When the autoshimming reaches the end criteria, the label on the STOP button automatically changes back to START.

On completion of shimming and/or locking operations, click the CLOSE button at the top of the screen to leave the acqi program. New parameter settings are written to the experiment at this time and normal acquisition is enabled again.

Shimming on the Lock Signal

When shimming on the lock, you monitor the intensity of the lock signal as you adjust the shim settings. Each shim setting controls the current through shim coils that control magnetic field gradients in different directions. It is important to know that the Z direction is parallel to the vertical direction of the probe and it is for this reason that the height of the sample in the NMR tube affects the Z shim settings rather dramatically.

1. The shim settings could be way off the mark (e.g., if the temperature has changed) and in this case the shim settings that have been most recently established for the particular probe you are using should be retrieved from the `shims` directory as a starting point.

   To retrieve the settings, enter `rts(file)`, where `file` is the name of a file containing the shim coil settings to be retrieved. `file` can be a name only (e.g., `rts('H1lshp')`), in which case the system searches for it, or it can be an absolute path (e.g., `rts('export/home/vnmr1/vnmrsys/shims/H1lshp')`). Refer to the description of `rts` in the *VNMR Command and Parameter Reference* for details on how the system searches for the file if you use only the file name.

   The `rts` command copies the shim settings in the file to the parameter set of the current experiment and sets `load='y'` to facilitate subsequent loading of shims with the `su` command (or other related commands).

2. Enter `su`.

   The `su` command sets up the system hardware to match the current parameters, including the shim settings you just retrieved, but does not initiate data acquisition. Now, if you make a change in a shim setting through the Acquisition window, that setting is retained until you change it by shimming again (using `acqi`), by entering another shim setting (like `z1=200`) followed by `load='y' su`, by using one of the autoshim methods, or by again retrieving a file of shim settings.

3. Make sure the probe has a sample, that it is spinning at the correct speed, and that the system is locked onto the deuterium resonance from the lock solvent.

4. Check that the lock signal is not saturated in the LOCK display window. The signal is saturated if you change the lock power by 6 units (6 dB) and the lock level changes by more than a factor of two. Set lock gain as necessary.
5. If the SHIM display window is not open, click the SHIM button from any Acquisition window to open it.

   In the SHIM display window, try a change of +4 or - 4 in the setting for Z1C. If the lock level goes up with one of these, continue in that direction until the level is maximized (it no longer increases, but instead begins to fall).

   At this time, if you are fairly certain your shim values are close to correct, you can click on the Z1C and Z2C (the coarse controls for Z1 and Z2) buttons until the signal level is maximized.
6. Change the setting for Z2C by +4 or - 4 and continue in that direction until the level is maximized.
7. Adjust Z1C for maximized lock level; then adjust Z2C for the same. Continue this iterative process until the lock level goes no higher. If the lock level increases to 100, decrease lock gain and then continue to adjust Z1C and Z2C. Lock power is adjusted by selecting z0/pwr/gn/ph from the SHIM menu. Return to the shims by selecting this shim window from the same SHIM window.
8. Adjust Z1 and Z2 (the fine Z controls) in the same way until the lock level is maximized.

In most cases, this concludes the shimming; however, some times it is necessary to shim the other Z controls and the non-spin shims. This must not be undertaken in the same way as the procedure above suggests. That is, if you simply go through Z1, Z2, Z3, and Z4 iteratively until the lock signal is maximized you may well find that your signal shape has degraded considerably. Hence, the following procedure is suggested for a second level of shimming:

1. After Z1 and Z2 have been adjusted for maximum lock signal, write down the lock level, adjust Z3 in one direction, say by +4, and then reoptimize Z1 and Z2 (iteratively) until the lock signal is at a maximum. Note this level of the lock signal. If the lock signal is higher than it was before (when you first wrote it down), continue changing Z3 in the same direction. Every change in Z3 must be followed by optimization of Z1 and Z2 until the lock level is at a maximum.
2. Repeat step 1 with Z4. That is, change Z4 in one direction, then optimize Z1 and Z2. If the lock level does not go up, change Z4 in the opposite direction and optimize Z1 and Z2. Continue until the highest possible lock level is obtained.
3. Repeat steps 1 and 2 iteratively until the highest possible lock level is obtained.
4. Turn the spinner off and go through the non-spin shims, one at a time, maximizing the lock level for each one. Then return and go through each again. Continue through all until the lock level is as high as possible. If lock is lost, increase the lock gain.
5. Turn the spinner on and optimize Z1 and Z2 as described above, return to the non-spins (turn the spinner off) and reoptimize these. Continue until the highest lock level is obtained.

For an ultimate check, you can now insert the lineshape sample ($CHCl_3$ in deuteroacetone for ^{1}H and dioxane in deuterobenzene for ^{13}C) and examine the line shape to make certain that you are close to the original specs, especially for the line shape at 0.55% and 0.11% of the total peak height. Also examine the height of the spinning sidebands. Refer to the *Acceptance Testing Procedures* manual for the system for measurement methods.

6.11 Shimming Using the Ultra•nmr Shim System

The Ultra•nmr Shims unit is a matrix shim system designed to achieve a high level of sample homogeneity over large sample volumes (e.g., 10-mm diameter), to generate more orthogonal shim gradients that are easier to use, and to provide this in a more reproducible and stable manner.

Ultra•nmr Shims are integrated with the UNITY*INOVA* system and all shim functions are available. Select the Ultra•nmr Shims from the CONFIG window or use the Ultra•nmr Console Data button in the window. The Ultra•nmr Shims unit can be connected to either port 2 of the console host CPU or PJ1 of the Magnet Sample Regulation (MSR) board. The MSR connection is preferred. If the interface box is present, the shims set by the console should be visible in its window, but the box should not be used.

CAUTION: **If an Ultra•nmr shim system can be controlled from the Acquisition window, do not set the shim value beyond ±32000 DAC counts.**

Hardware Overview

The system uses a matrix of 48 channels to provide current into 49 coils within the room-temperature shim tube from which 38 or 39 shim gradients are generated. Each of the axial shim gradients is produced by applying currents simultaneously in up to 12 different channels, and each of the radial gradients, in up to 6 different channels with the 48-channel matrix system. The distribution of current within the allowed channels for each gradient is under computer control and is calibrated to produce the purest (most orthogonal) possible single shim gradient. For example, the distribution of current for the Z2 gradient is adjusted so that the Z2 gradient produced has minimal amounts of other gradients, such as Z (=Z1) or Z0.

An interface box provides five user-selectable, optically encoded knobs to control the shim gradients. The interface box also provides the user with a means of storing, viewing, and recalling up to 63 shim sets on a floppy disk. Each of the shim gradients has both coarse and fine controls, with each control having a range of ±32767 DAC counts. The following gradients are controlled:

Axial:	Z0, Z, Z2, Z3, Z4, Z5, Z6, Z7, Z8
Radial:	X, ZX, Z2X, Z3X, Z4X, Z5X
	Y, ZY, Z2Y, Z3Y, Z4Y, Z5Y
	C2, ZC2, Z2C2, Z3C2, Z4C2 (where C2 = XY)
	S2, ZS2, Z2S2, Z3S2, Z4S2 (where S2 = X2Y2)
	C3, ZC3, Z2C3, Z3C3 (where C3 = X3)
	S3, ZS3, Z2S3, Z3S3 (where S3 = Y3)

Interface Box

The interface box (see Figure 48) has a small display screen and the following controls:

- Five knobs whose gradient assignments are selected by toggle switches.
- Two identical toggle switches, each labeled YES/NO.
- Eight buttons: MODE, BANK, FILE, LOAD, VIEW, STORE, DRIFT, and C/F. A small indicator above each button turns green if the button is active.

The MODE, BANK, and FILE buttons select the system mode:

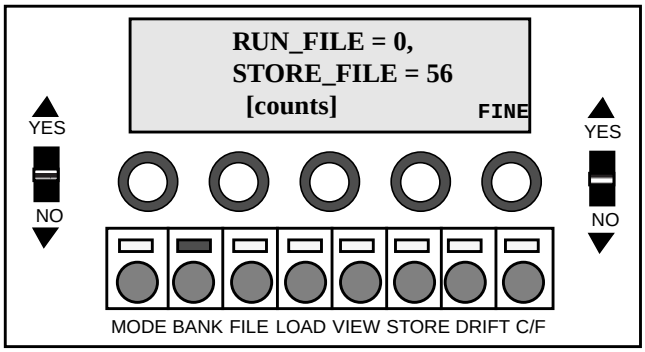


Figure 48. Ultra•nmr Shim. System Interface Controls and Display

- MODE mode allows the user to reconfigure the system and the display screen by using the toggle switches to select configuration options.
- BANK mode makes shim gradient control accessible through the knobs. In this mode, the toggle switches select banks of knob-to-gradient assignments, which are displayed on the display screen directly above the knobs.
- FILE mode lets the user load from, view, or store to whichever STORE_FILE file number is selected by the toggle switches. These file actions are initiated by the LOAD, VIEW, or STORE buttons, respectively. Immediately after any LOAD or STORE operation, the RUN_FILE and STORE_FILE file numbers are identical. If any changes are subsequently made to the existing gradient DAC values, RUN_FILE is reset to 0.

The last button on the right, the coarse/fine gradient control (C/F) button, is active in both the BANK and the FILE modes.

Files 2 through 63 are available for user storage. Users can *not* write to file 0, which contains all zeros, or write to file 1, which contains converged shim values. Files are stored on a DOS-formatted 1.4-MB floppy disk in a drive accessible from the front of the main unit. The small cover panel at the right edge of the upper card cage must be removed to gain access to the system floppy disk. New disks must be formatted using DOS version 5.0 or higher. Numerous calibration files will be copied to that disk. Copies of existing floppy disks can be made using the DOS `diskcopy` command on any machine running DOS version 3.3 or higher; for example, enter `diskcopy a: a:` if the particular floppy drive is configured to be drive A.

One of the selectable options in the MODE mode allows system lock out for security reasons. If this feature is activated, all knob, button, and toggle control is disengaged until the MODE, BANK, and VIEW buttons are simultaneously pressed. It is also possible to disable (turn off) the lock from the interface box in the MODE mode. This feature is contained in the Z0 enable/Z0 disable option.

After Ultra•nmr Shims are installed, Z0 is not controlled via the Acquisition window but only from the Ultra•nmr Shims interface box. All other lock parameters—`lockpower`, `lockgain`, and `lockphase`—remain controlled through the Acquisition window. The value of Z0 changes about +3500 coarse DAC units on a 500-MHz magnet (about +4200 on a 600-MHz magnet) when the lock solvent changes from $CDCl_3$ to acetone-d_6. The other shim gradients are also no longer controlled through the Acquisition window.

Homospoil (Z gradient) produces approximately a 0.6 G/cm field (typically 99% of transverse magnetization is gone within 1.5 ms and signal recovery is 90% within 40 ms) and is activated in the same manner as a spectrometer linked to Oxford room-temperature shims.

Shimming

In the normal “counts” display mode, each shim gradient has a coarse and a fine control. The coarse control is 50 times more sensitive than the corresponding fine control. All gradient DACs have a range of ±32767; a knob twisted beyond this range will continue to turn but have no effect. Each of the gradient DACs has an identical and a logical polarity. For example, a clockwise adjustment of Z2 moves an asymmetry to the right, with Z2 coarse (Z2C) and Z2 fine moving asymmetries in the same direction. Furthermore, Z4, Z6, and Z8 also move asymmetries in the same direction as Z2. The even-order axial shims (Z2, Z4, Z6, and Z8) may jerk the lock if large, sudden changes are made; the severity of the jerk decreases typically in the order Z4, Z8, Z2, and Z6.

Within gradient families, you also observe sensitivity differences, with higher order gradients causing less effect per DAC unit. The following suggestions are offered:

- Z0: use coarse only (fine is too fine).
- Z: use fine only (coarse is *far* too coarse).
- Z2, Z3, Z4: use coarse or fine, whichever seems best.
- Z5, Z6, Z7, Z8: use coarse only.
- Radial shims: use coarse, with the possible exception of X and Y.

Remember that the gradients produced are purer (more orthogonal) so shimming methods subjectively generated on other shim systems may not behave the same. If you adjust any axial shim, you should probably touch up Z before touching any other gradients (for example, if you change Z4, then optimize Z before touching up Z2). In addition, be forewarned that 80% of what might be corrected with Z4 using an Oxford shim system is probably corrected with Z2 when using Ultra•nmr Shims.

Installing the First Probe

Starting from the final converged results obtained with field mapping, it is possible to obtain a lineshape of less than 7/12 Hz (non-spin) in under an hour or two on 1% $CHCl_3$ in acetone-d_6 (ASTM ^1H lineshape sample). Z and Z2 typically change the most (Z fine needs about –70 units, Z2 about –400 units), but Z3, Z4, Z5, X, and Y will need adjustment. The higher-order radial shims are typically converged to a better value than a user can determine spectroscopically and should therefore not be adjusted manually (only X, Y, ZX, ZY, and possibly C2 and S2 should need adjustment). A simple maximization of the lock level has proven to be a sufficient criterion.

Floppy Disk Use

Every Ultra•nmr Shims floppy should contain 83 system files and up to 62 user files. The system files include 39 strength files (`*.str`), 39 divider files (`*.div`), a gradient-channel configuration file (`*.him`), a shim-coil resistance file (`*.res`), a shim configuration file (`*.cfg`), and two shim files (`file0.dac` and `file1.dac`). `file1.dac` is to contain the shim values for the $CHCl_3$ lineshape sample in one particular probe. The 62 user files are the shim files 2 to 63 (`file#.dac`).

A version of each of the system files is stored in the system PROM (programmable read-only memory). If any system file is missing on the floppy disk, the PROM version is used instead. It is acceptable to use the PROM versions for the `*.him`, `*.res`, and `*.cfg` system files. It is *not* acceptable to use the PROM versions for the `*.div` and `*.str` files because these files are set at the time of system installation and are magnet dependent.

The `readultra` macro reads shim set files for the Ultra•nmr shim system from a floppy disk on a Sun workstation into VNMR (e.g., entering `readultra(6)` reads shim set file 6). Entering `readultra` with no argument reads all of the shim set files. Before using `readultra`, the floppy disk is expected to be mounted as `/pcfs` on the Sun workstation. For details, refer to the description of `readultra` in the *VNMR Command and Parameter Reference*.

In a multiuser environment, it is probably best if each user has a separate floppy disk on which that user's particular shim files can be written. In any environment, backup floppy disks are always a good idea. Two backup system disks are made at the time Ultra•nmr Shims is installed: one is to be kept by the customer; the other is sent to Varian. Backup disks can be easily made on any DOS-based computer using the DOS `diskcopy` command.

CAUTION: **Keep floppy disks away from the magnet dewar. Data on the disk is susceptible to damage from intense magnetic fields.**

When changing floppy disks, observe the following procedure:

1. Save the current shim values into one of the 62 available shim files.
2. Load in file 0.
3. Remove the current floppy from the drive and immediately insert the new system floppy into the drive. *Do not operate the controls on the interface box when there is no floppy in the drive*.

Enabling the Acquisition Window

The shims can be controlled with the Acquisition window instead of from the interface box. To enable software control, press the Mode button on the interface box to activate the mode select feature. Use the NO direction on the YES/NO toggle switch to toggle through to display RS232 TERMINAL MODE on the interface display screen. Toggle the YES/NO switch to the YES position to select the serial mode. The interface box screen will display RS232 TERMINAL MODE ENGAGED. To revert to the manual mode, push the Mode button and then the Blank button on the interface box.

Turning the System Off and On

The system is typically left on continuously except for maintenance.

To Turn Off the System

Use the following procedure to power down the Ultra•nmr Shims system:

1. Save the current shim values into one of the 62 available shim files.
2. Load in file 0.
3. Turn off the orange-lighted rocker switch on the power strip in the lower back of the shim power supply.

To Turn On the System

Use the following procedure to turn the shim system back on:

1. Press the rocker switch on the power strip The orange light in the switch should turn on and the interlock board in the bottom left front of the shim power supply should

display two red lights and one green light. The bootup of the computer in the shim power supply takes approximately one minute. During the bootup, all eight indicators, situated above the eight buttons on the interface box, are usually lighted green. Note that the system will not boot unless a readable floppy disk is in the system floppy drive.

When the bootup is complete, the interface box displays several status messages indicating how many PROM-based default files were used during bootup.

2. When the final question is displayed on the interface box, you must answer “yes” before the high-power interlock is disengaged.

When the high-power interlock disengages, one of the two red lights previously displayed at the front of the interlock board turns off. It is *perfectly normal* for the other red light to stay on all the time.

6.12 Gradient Autoshimming

Gradient autoshimming provides rapid, automatic adjustment of room-temperature shims. It is a very reliable way to set high-order shims, eliminating many hours previously spent on shimming. Typical gradient autoshimming time is only a few minutes, and all steps are done with a few clicks of a mouse button.

Gradient autoshimming is implemented for use with the axial gradients (Z-gradients). For optimal gradient shimming, a PFG amplifier and probe are recommended for their fast recovery performance. However, if a PFG amplifier and probe are not available, gradient autoshimming can be performed using the homospoil gradients (Z1 room temperature shim coil). For more details on how to set up homospoil gradients, refer to “Homospoil Gradient Type” in the chapter on PFG modules operation in the manual *User Guide: Liquids NMR*.

Gradient autoshimming methods support shimming on a wide variety of samples with different volumes and solvents. For aqueous samples, water protons provide sufficient signal for shimming. For deuterated solvents, gradient shimming can be performed if there is sufficient deuterium signal. Deuterium gradient shimming is feasible on most samples where the lock solvent is a single, strong resonance, which includes the majority of solvents of interest for routine NMR use.

Proton gradient autoshimming with PFG is available on all systems configured with a PFG accessory. Deuterium gradient shimming is only available on UNITY*INOVA*, UNITY*plus*, *MERCURY-VX*, and *MERCURY* systems and not on *GEMINI 2000*, UNITY, and VXR-S systems, because lock sample and hold capability is required to perform deuterium gradient shimming. A hardware upgrade is also required to perform deuterium gradient shimming. System configuration requirements are summarized in Table 21.

Table 21. Gradient Shim Availability

System	*Gradient Shim Availability*
UNITY*INOVA*, UNITY*plus*	^{1}H or ^{2}H with PFG or Homospoil[a]
MERCURY-VX, *MERCURY*	^{1}H or ^{2}H with PFG or Homospoil[b]
UNITY, VXR-S, *GEMINI 2000*	^{1}H with PFG only

a. Automated deuterium gradient shimming module required for deuterium gradient shimming with PFG or homospoil.
b. Automated liquids/solids spinner controller and automated deuterium gradient shimming module required for deuterium gradient shimming.

Gradient Shimming Method

The gradient shimming method uses a pair of gradient profile-type experiments to calculate the B_0 field, and make appropriate corrections to the shims. The pulse sequence and calculation are described in detail in the chapter on PFG modules experiments in the manual *User Guide: Liquids NMR*. The full gradient shimming method has these steps:

1. Map the shims.
2. Perform autoshimming.

The shims must be mapped before autoshimming is used. Mapping the shims is necessary when a new probe is installed, but can be repeated at any time.

Table 22 summarizes gradient shimming commands and parameters.

Table 22. Gradient Shimming Commands and Parameters

Commands	
`dg2`	Display group of parameters.
`gmapshim<('files'|'quit')>`	Run gradient autoshimming, get files and parameters, quit.
`gmapsys*`	Enter Gradient Shimming System menu, make shimmap.
`gmapz<(mapname)>`	Get parameters/files for `gmapz` pulse sequence.
`* gmapsys<'shimmap'<,'auto'|'manual'|'overwrite'|mapname>`	
Parameters	
`gradtype*`	Gradients for x, y, and z axes
`gzlvl {DAC value}`	Pulsed field gradient strength
`gzsize {integer,1 to 8}`	Number of z-axis shims used by gradient shimming
`gzwin {0 to 100}`	Percentage of spectral window used by gradient shimming
`pfgon{'nny'` if on}	PFG amplifiers on/off control
`*` `gradtype` {3-character string from `'n','w','l','p','q','s','t','u','h'}`	

Configuring Gradients and Hardware Control

1. Confirm that PFG or homospoil gradients are installed on your system. See the chapter on PFG modules experiments in the manual *User Guide: Liquids NMR*.
2. Confirm that the gradients are active by checking that `gradtype` and `pfgon` are set appropriately for your system. Use `config` to change settings if necessary.
3. If you have the Ultra•nmr shim system, enable control of the shims from the Acquisition window, as described in section “Shimming Using the Ultra•nmr Shim System” on page 164.

CAUTION: **Do not spin the sample during gradient shimming. Spinning may cause motion artifacts.**

Mapping the Shims

Mapping the shims is necessary after installing a new probe. 90% H_2O is recommended for first time shimming on ^1H and 1%H_2O/99%D_2O is recommended for ^2H.

1. Insert a sample and find lock.
2. Stop sample spinning (**`spin=0`**). Disable sample changer control (**`loc='n'`**).
3. Adjust lock power, lock gain, and lock phase. Make coarse shim adjustments on Z1, Z2, X1, and Y1.

4. Use **s2pul** to find the 90° pulse for `tn='H1'` or `tn='lk'`, as appropriate.
5. Enter **gmapsys** to display the Gradient Shimming System menu.

   Standard parameters are retrieved from `gmapz.par` the first time `gmapsys` is entered, or if a shimmap was previously made, parameters are retrieved from the current shimmap. If desired, enter **gmapz** to retrieve standard parameters from `gmapz.par`.
6. To set parameters for a particular gradient and nucleus, enter **gmapsys** and click on **Set Params > Gradient, Nucleus**, and then click on the appropriate button (**Pfg H1, Pfg H2, Homospoil H1,** or **Homospoil H2**). Next, set pw as follows:
   - For PFG, set **pw** to the 90° pulse or less.
   - For homospoil, set **pw** to 90° pulse and `p1` to 180° pulse.
7. Test the parameters. Enter **gmapsys** and click on **Set Params** > **Go, dssh**.

   You should see two profile spectra. If you don't, check that the gradients are active and check `pw`, `tpwr`, and `gain`.
8. To make a shimmap, again enter **gmapsys** and click on **Shim Maps** > **Automake Shimmap**. Enter a mapname (any string valid for a file name) at the prompt.

Automake Shimmap first runs an experiment that calibrates `gzwin` and `tof` to set the spectral window. Next, it runs an experiment with the shims arrayed to map the shims, and processes the experiment when done. Coarse shims are used if present. The parameters and data for the shimmap are stored in the file `userdir + '/gshimlib/shimmaps/' + mapname + '.fid'`. These parameters are retrieved the next time gradient shimming is run if the gradient shimming system menu is exited.

To begin shimming, skip to "Automated Shimming" on page 172.

Displaying the Shimmap

After the shims are mapped, display the shimmap by entering `gmapsys` and clicking on **Display > Display Shimmap**. The shimmap display is a multicolored plot of the shimmap, with Z1 as #1 and Z2 as #2, and so on (see Figure 49).

The shimmap is specific to the probe used, and can also be dependent on sample volume for small volumes. The shimmap shows the actual field dependence of the shims, except for a dc offset added for display purposes. Good signal-to-noise in the shimmap is needed for the shimming to work well. Poor signal-to-noise may result in misset shims.

Calibrating gzwin

The parameter `gzwin` is the percentage of the spectral window used in calculating the field maps. `gzwin` should be adjusted only when making a new shimmap. If this parameter is not calibrated correctly, you may see excess noise data at the edge of the shimmaps, which corresponds to the region in the profile spectrum where the signal goes to zero. It is normal to have a few noise data points at the edge of the shimmap, but if it is more than a few data points (greater than 25% of the window), `gzwin` may be miscalibrated. This can occur if there is low signal-to-noise or if `gzwin` has not previously been calibrated for the current parameter set. If the gain is too high, "wings" will appear on the sides of the spectra and may result in miscalibrated `gzwin`. This can also occur if there are multiple chemical shifts in the presence of a weak gradient.

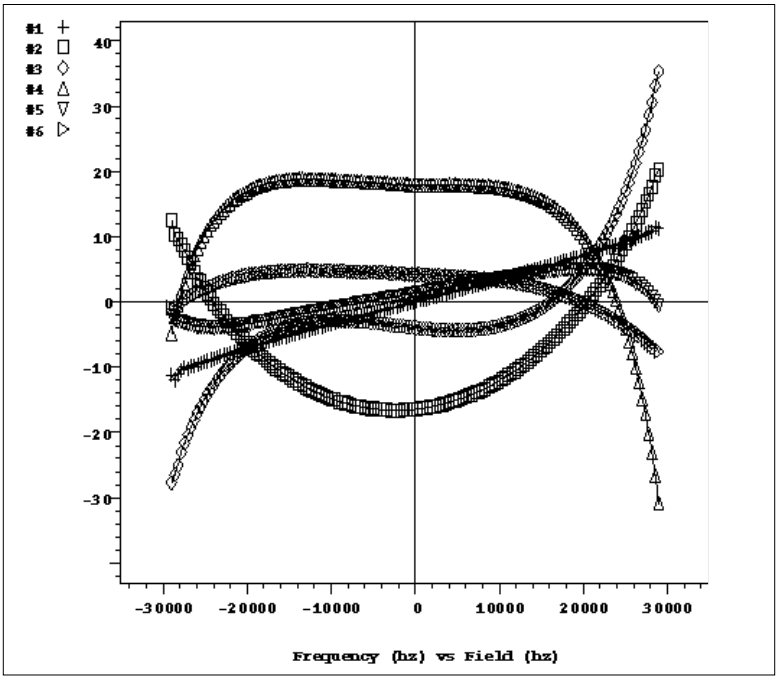


Figure 49. Shimmap Plot

Automatic Calibration of gzwin

Clicking the Automake Shimmap button causes the following actions:

1. Enter **gmapsys** and click on **Set Params** > **Find gzwin**, which calibrates `gzwin` and sets `tof` to center the window used for calculation.
2. Click on **Return** > **Shim Maps** > **Make Shimmap**, which makes the shimmap with the current values of `gzwin` and `tof`.

You may click through these steps separately to see if `gzwin` is calibrated correctly. The box cursors at the end of step 1 should be at either edge of the profile.

Manual Calibration of gzwin

Manual calibration of `gzwin` may be used to avoid noise spikes in the spectrum, or other artifacts. To manually calibrate `gzwin`, do the following:

1. Click on **Set Params** > **Go, dssh**. Wait until the experiment is done.
2. Enter **ds**, and set the box cursors near the edges of the profile.
3. Enter **gmapsys**, and click on **Set Params** > **Calculate gzwin**.
4. Click on **Return** > **Shim Maps** > **Make Shimmap**.

The parameter `gzwin` should be adjusted only when making a new shimmap. The calibrated value of `gzwin` is saved when the new shimmap is saved at the end of the mapping experiment. The same value of `gzwin` must be used in shimming as in making a shimmap, and should not be adjusted when shimming.

Shimmap Files and Parameters

The parameters and shimmap files saved under a mapname are retrieved when that mapname is retrieved. When reinserting a probe, reload the shimmap for that probe. If you are unsure if the shimmap is correct, make a new shimmap, which typically only takes a few minutes. The last parameters and files used are automatically retrieved the first time `gmapsys` is entered. If `gmapsys` is entered again, the parameters are not retrieved. Gradient shimming uses the current parameters after the pulse sequence is loaded (`seqfil='gmapz'`).

Standard parameters can be loaded before making a shimmap by entering `gmapz` or by using the **Gradient,Nucleus** menu button. Parameters and files can also be explicitly loaded and distributed, as described in the following subsections:

Loading a Shimmap

To change shimmaps as a system administrator, do the following:

1. Enter **`gmapsys`**.
2. Click on **Shim Maps** > **Shimmap Files** > **Cd to Userdir**.
3. Select a file.
4. Click on **Load Shimmap** (loads the shimmap files `gshim.list` and `gshim.bas` from `gshimlib/shimmaps/mapname.fid` into `gshimlib/data`, but does not load the parameters) or click on **Load Shimmap & Params** (loads shimmap files and parameters).

The general user can also change shimmaps by entering **`gmapshim('files')`** from any experiment to display the Gradient Autoshimming Files menu, and then clicking on either the **Load Shimmap** or **Load Shimmap &Params** buttons.

Distributing a Shimmap

The system administrator can copy a shimmap file from `vnmrsys/gshimlib/shimmaps` into the directory `/vnmr/gshimlib/shimmaps` so that the file is accessible to all users. To copy files, do the following steps:

1. Enter **`gmapsys`**.
2. Click on **Shim Maps** > **Shimmap Files** > **Cd to Userdir**.
3. Select a file.
4. Click on **Copy to Systemdir**. You must be `vnmr1` for this button to appear.

Automated Shimming

The shims must be mapped before gradient autoshimming is used. See “Mapping the Shims” on page 169 for details.

Starting Gradient Shimming

To start shimming from the system administrator menu, enter **`gmapsys`** and then click on **Autoshim on Z**. This button starts gradient shimming using current parameters, and displays the curve fit for each iteration. The curve fit plot shows the raw data as #1 and the curve fit as #2 (see Figure 50).

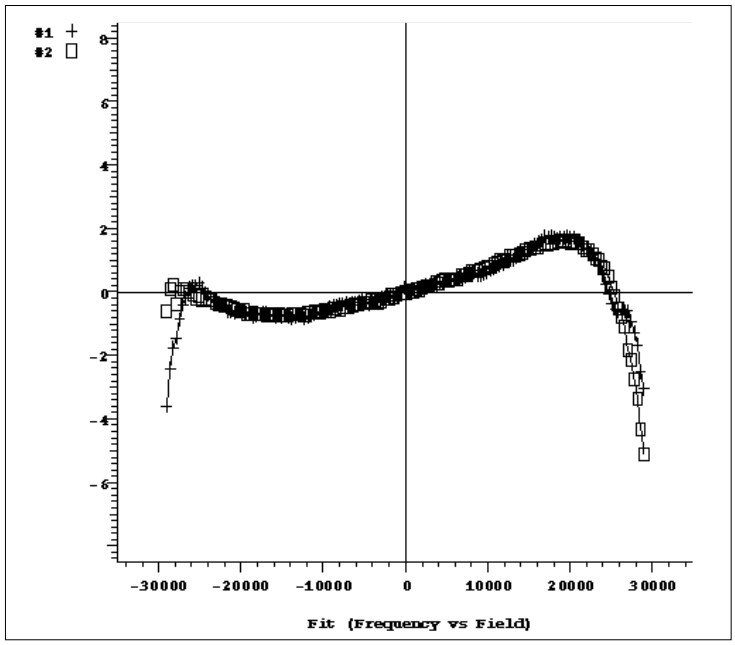


Figure 50. Curve Fit Plot

Shim adjustments for each iteration are also displayed (see Figure 51) and have converged when the rms error number is less than 1.0. Gradient shimming continues until convergence or until a maximum of 10 iterations are reached.

```
mapname 5mm_Triax_01
shimset 4  gzsize 6                          rms err 1.892

Shim    Offset     Old      New        Diff      Error
-------------------------------------------------------------
z1      800        -9405    -9269      -136      48
z2      800        -3118    -3104      -14       13
z3      3200       -4356    -4321      -35       37
z4      -3200      4049     4885       -836      104
z5      -3200      13443    14537      -1094     322
z6      3200       -15619   -12568     -3051     467
z7      3200       0        0          0         0
z8      3200       0        0          0         0
-------------------------------------------------------------
```

Figure 51. Display of Shim Adjustments for Each Iteration

If a shim goes out of range, the shim is set to maximum and shimming continues with the remaining shims. If convergence is then reached, shimming is tried once more with all Z shims and continues unless a shim goes out of range again.

If the parameter `gmap_z1z4` is set to `'y'`, then if `gzsize` is greater than 4, shimming is done first on Z1–Z4 and then proceeds with all shims specified by `gzsize`. Gradient shimming takes longer and goes through more iterations, but this may avoid the problem on some systems where a high-order shim (i.e. Z5, Z6) goes out of range because it contains impurities from lower-order shims. This parameter may be set at any time while shimming

from gmapsys. In order to use this parameter in user autoshimming, set it before making a shimmap, or in the corresponding parameter set in gshimlib/shimmaps.

Quitting the Gradient Shimming System Menu

Enter **gmapsys** and click on **Quit** to exit from the gmapsys menu system. This also retrieves the previous parameter set and data, including any data processing done on the previous data set.

Deuterium Gradient Shimming

Deuterium gradient shimming is feasible for most deuterated solvents because the lock solvent usually has a single, strong deuterium resonance with sufficient signal.

The automated deuterium gradient shimming module is required to run deuterium gradient shimming. If present, this module automatically holds the lock at its current value and switches the transmitter cable to pulse the lock coil when an experiment is run with tn='lk'. The module is strongly recommended for all users who wish to run deuterium gradient shimming in automation. See Table 21 for system configurations supported.

The system administrator must make a shimmap on deuterium before deuterium gradient shimming can be used. Follow the procedure “Mapping the Shims” on page 169 using the deuterium signal for all steps, (use tn='lk' for step 4, and select **Pfg H2** at step 6). The transmitter power (tpwr) should be kept low to avoid probe arcing, with a 90° pulse greater than about 200 µs.

Deuterium gradient shimming is recommended for shimming in automation with different solvents. The system administrator should also uncomment the section in the gmapz macro, which sets parameters based on solvent, similar to the section of the setlk macro. The gmapz macro may be customized for particular applications. Table 23 summarizes the recommended parameters for some common deuterated solvents.

Table 23. Typical ^{2}H Gradient Shimming Parameters for Common Solvents

Solvent	*nt*	*d1 (sec)*
deuteroacetone	4	6-12
D_2O	4	3
deuterobenzene	4	3
dmso-d6	16	3
deuterochloroform	64	3

The deuterium parameters are saved for future use when the shimmap is saved, and are used the next time gradient autoshimming is run.

Homospoil Gradient Shimming for ^{1}H or ^{2}H

It is also possible to use the Z1 room temperature shim as a homospoil gradient, instead of using a pulsed field gradient or PFG. Use of this option is recommended only if a PFG amplifier or probe is not available. For details on how to configure a homospoil gradient, see the section “Homospoil Gradient Type” in the chapter on PFG modules operation in the manual *User Guide: Liquids NMR*. The system administrator must make a shimmap using homospoil before homospoil gradient shimming can be used. Follow the procedure in “Mapping the Shims” page 169.

At step 4 select tn as appropriate, set tof on resonance, and then find the 90° pulse. If deuterium is used, tpwr should be kept low, with a 90° pulse greater than about 200 µs.

At step 6, select either **Homospoil H1** for proton parameters or **Homospoil H2** for deuterium parameters, as appropriate. Homospoil gradients must be configured at this step (use `config` or set `gradtype='nnh'`).

At step 7, further testing of the gradient shimming parameters for homospoil can be done as follows:

1. Enter **`gmapsys`**, and click on **Set Params** > **Go,dssh**.
2. Using the 90° pulse from step 4, calibrate the 90° and 180° pulses to obtain an echo. Enter **`df`** to display the FID. You should see an echo forming in the middle of the FID.
3. If needed, adjust **`sw`** so that the gradient covers at least 10% of the spectral window. Increase **`np`** to 512 to improve Hz/point resolution. However, `np` should be adjusted so that `at` is not longer than the homospoil time limit (20 ms on standard UNITY*INOVA* and UNITY*plus* and 200 ms with the automated deuterium gradient shimming module). The acquisition time (`at`) should also be shorter than T_2. Set **`d2=at/4`**.

Once all the parameters are set, click on **Automake Shimmap** (step 8). The parameters are saved when the shimmap is done and are used the next time gradient autoshimming is run.

To use homospoil deuterium gradient shimming with different solvents, set the parameter **`gmap_findtof='y'`**. This should be done before making the shimmap, or may be set in the corresponding parameter set in `gshimlib/shimmaps`. Gradient shimming will then perform a calibration to find tof before autoshimming starts. This takes an extra iteration in the shimming procedure, but is essential for homospoil deuterium gradient shimming to function correctly in automation.

Full Deuterium Gradient Shimming Procedure for Lineshape

The automated deuterium gradient shimming module must be installed to use this procedure.

1. Insert the appropriate lineshape sample (chloroform in acetone-d6) and find lock. Turn off spinning and disable sample changer control. Adjust lock power, lock gain, and lock phase as necessary. Do quick shimming on z1, z2, x1, y1 (use z1c, z2c, if present).
2. Find the 90° pulse on ^{2}H as follows:
   a. Enter **`s2pul tn='lk' tpwr=42 pw=200`**.
   b. Enter **`ga`** and wait for acquisition to finish. You should see only a single line. Place the cursor on resonance and enter **`nl movetof`**.
   c. Enter **`array('pw',20,100,100)`**. Enter **`ga`** and wait for acquisition to complete.
   d. Set `pw90` to the first maximum.
3. Set up gradient shim parameters. Enter **`gmapsys`** and click on **Set Params** > **Gradient, Nucleus**.
   a. If you have PFG, click on **Pfg H2**, set **`pw`** to one half the 90° pulse found in step 2 and set **`d1=6`**.
   b. If you have homospoil, click on **Homospoil H2**, set **`pw`** to the 90° pulse, **`p1`** to the 180° pulse, and **`d1=6`**.
4. Enter **`gmapsys`**, click on **Set Params** > **Go,dssh**, and wait for acquisition to complete. You should see two profile spectra.

5. Map the shims. Enter **gmapsys** and click on **Shim Maps** > **Automake Shimmap**. At the mapname prompt, enter a file name. Wait for acquisition to complete and the message to be displayed: `shimmap done`!
6. Perform shimming on z's. Enter **`gmapsys`** and click on **Autoshim on Z**. Wait for the acquisitions to complete, and the message to be displayed: `Gradient Autoshimming on Z done! N iterations`.
7. Enter **`acqi`** and adjust lock phase. Shim only on low-order nonspins (x1, y1, xz, yz, etc.). Do not shim on z's (z1, z2, etc.).
8. Perform shimming on z's. Repeat step 6.
9. Measure proton lineshape. Turn on spinner if appropriate, and enter **`acqi`** to make fine shim adjustment. Shim on all shims as necessary.

General User Gradient Shimming

For the general user, gradient shimming can be run from outside `gmapsys` from any experiment. Any one of the following methods is recommended for routine use:

- Click on **Main Menu** > **Setup** > **Shim** > **Gradient Autoshim on Z**. Parameters are retrieved from the current mapname, which is displayed at the start of shimming, and the spinner is automatically turned off. The curve fit and shim adjustments are not displayed. The previous parameter set and data are retrieved when shimming is finished. This button only functions after a shimmap is made.
- Enter **`gmapshim.`** This performs the same action as clicking on **Gradient Autoshim on Z**.
- Within automation parameter sets, use **`wshim='g'`** (UNITY*INOVA*, *MERCURY-VX*, UNITY*plus*, and *MERCURY* only).

To stop gradient shimming before it is completed, use one of the following methods:

- Click on **Main Menu** > **Setup** > **Shim** > **Quit Gradient Shim**. Quitting aborts the experiment and retrieves the previous parameter set and data.
- Enter **`gmapshim('quit')`**. This performs the same action as **Quit Gradient Shim**.
- Abort the acquisition with **`aa`** and click on **Cancel Cmd**. Then enter **`gmapshim('quit')`** to retrieve previous data set and parameters.

Suggestions for Improving Results

Calibrate the 90° pulse and adjust `tpwr`, `pw`, and `gain` to optimize signal-to-noise. Reduce gain if ADC overflow occurs, which may appear as wings on the profile.

For solvents with long T_1, set `d1` to 3 to 5 times T_1, or use a small flip angle for `pw`. Stimulated echoes may otherwise result, which may appear as excess noise or a beat pattern in the spectrum, or as secondary echoes in the FID (use `df` to observe this).

The phase encode delay `d3` is arrayed to two values, the first of which is zero. The second value can be increased for better signal-to-noise in the phase maps, up to about the point where the amplitude of the second profile is half that of the first (about 2/3 T_2 without radiation damping; radiation damping can be severe in water ^{1}H). However, longer `d3` values increase the phase excursion, and can make it difficult to shim large shim corrections (especially Z1). Typical ^{1}H values are 5 to 30 ms, and typical ^{2}H values are 30 to 200 ms.

When reinstalling a probe, make sure it is in the same vertical position in the magnet barrel as when the shimmap was made. If you are unsure, make a new shimmap, which typically takes only a few minutes.

Alternate between z-axis gradient shimming and shimming the low-order x- and y-axis shims by other methods (e.g., on lock level). The z-axis shims account for the majority of sample volume changes (changes in height), and the x- and y-shims are relatively insensitive to change in height. Evaluate shimming for a particular application, since the ideal lineshape may vary with the application.

The high-order shims can sometimes be set off-scale during shimming. This may occur if the sample is short, or if the sample is improperly seated in the probe, or if the high-order shims are weak. In such cases, the off-scale shim is set to maximum, and shimming continues with lower-order shims. Superior results can be obtained in some cases by first setting `gzsize=4` and clicking on Autoshim on Z to shim on `z1`–`z4`, and then shimming the low-order transverse shims, and then increasing `gzsize` and shimming again. This may also be done using `gmap_z1z4='y'`. On a short sample it also can be useful to remap the shims.

Some shim systems may need additional time when running the shim mapping experiment to allow the shims to settle. The added time is especially noticeable on some systems for Z4. To account for added time, lengthen the `d1` delay or add dummy scans in between each array element (e.g., `ss=-2`). Decreasing the amount a shim is offset also allows the shim to settle more quickly. Enter `gmapsys('vi')` to edit the values in the Offset column, and then enter `gmapsys('shimmap','manual')` to map the shims with user-defined offsets. A new mapname may also be set using `gmapsys('vi')`.

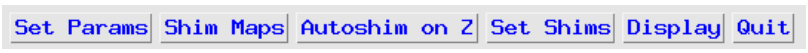
Coarse shims are used on systems on which they are available. To use fine shims on these systems, enter `gmapsys('vi')` to edit the entries in the shim column (e.g., change `z1c` to `z1`), and then enter `gmapsys('shimmap','manual')` to map the shims.

For samples in H_20, the water protons provide sufficient signal for shimming. For samples other than water, deuterium gradient shimming is strongly recommended if there is sufficient deuterium signal. Proton gradient shimming can be made to work in samples other than water if there is sufficient proton signal and the signal is well-resolved (does not overlap with other strong resonances). Gradient shimming can also be done on a water sample of equal height of the sample of interest, and then the sample of interest can be inserted.

For further information, refer to the entries for `gmapshim`, `gmapsys`, and `gmapz` in the *VNMR Command and Parameter Reference*.

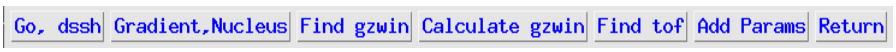
Gradient Shimming Menus

The top-level gradient shimming menu is the Gradient Shimming System menu, which is opened by entering `gmapsys`.



From this menu and submenus, there are buttons to open the following menus:

- Gradient Shimming Setup menu



- Gradient Nucleus Parameter Setup menu

- Gradient Shimming Map menu

- Gradient Shimming Files menu

- Gradient Shim Setting menu

- Gradient Shimming Display menu

- Gradient Shimming Plot menu

Two other gradient shimming menus are available for the general user:

- Automated Shimming menu. To open, click on Main Menu | Setup | Shims.

- Gradient Autoshimming Files menu. To open, enter `gmapshim('files')`.

A description of each menu (in the same order as above), the button or command for opening the menu, and the action of each button in the menu is given in the following sections. On all menus, the left mouse button is used to click on the desired choice in the menu. The other mouse buttons are not active.

Gradient Shimming System Menu

The Gradient Shimming System menu is the top-level menu for gradient shimming setup and shim mapping. To open this menu, enter `gmapsys`.

Button	*Description*
Set Params	Enter Gradient Shimming Setup menu.
Shim Maps	Enter Gradient Shimming Map menu.
Autoshim on Z	Start gradient shimming using current parameters. Fit is displayed with each iteration.
Set Shims	Enter Gradient Shim Setting menu.
Display	Enter Gradient Shimming Display menu.
Quit	Return to previous experiment.

Gradient Shimming Setup Menu

The Gradient Shimming Setup menu is used for calibrating gradient shimming parameters. To open this menu, click on Set Up in the Gradient Shimming System menu.

Button	*Description*
Go, dssh	Run and display profile spectra.
Gradient,Nucleus	Enter Gradient,Nucleus parameter setup menu.

Button	*Description*
Find gzwin	Run a calibration experiment to set parameters `tof` and `gzwin`, to optimize the spectral window for a given `gzlvl`. Pulse length and gain should be correctly set before using this button.
Calculate gzwin	Determine `tof` and `gzwin` from the profile spectrum using cursor positions.
Find tof	Run a calibration experiment to set tof. Pulse length and gain should be correctly set before using this button
Add Params	Add parameters for gradient shimming.
Return	Return to the Gradient Shimming System menu.

Gradient Nucleus Parameter Setup Menu

The Gradient Nucleus Parameter Setup menu is used for setting parameters according to type of gradient and nucleus. Recabling may be required to observe ^{1}H or ^{2}H nucleus. Check the value of `gradtype` when done. To open this menu, click on Gradient,Nucleus in the Gradient Shimming Setup menu.

Button	*Description*
Pfg H1	Set parameters for pulsed field gradient on ^{1}H.
Pfg H2	Set parameters for pulsed field gradient on ^{2}H.
Homospoil H1	Set parameters for homospoil gradient on ^{1}H.
Homospoil H2	Set parameters for homospoil gradient on ^{2}H.
Return	Return to the Gradient Shimming Setup menu.

Gradient Shimming Map Menu

The Gradient Shimming Map menu is used for making and retrieving shimmaps. To open this menu, click on Shim Maps in the Gradient Shimming System menu.

Button	*Description*
Automake Shimmap	Find `gzwin` and then run shimmap experiment.
Make Shimmap	Run shimmap experiment.
Shimmap Files	Enter Gradient Shimming Files menu.
Current Mapname	Show current mapname used for gradient shimming.
Save As	Save current parameter set and shimmap files. Enter mapname when prompted.
Return	Return to the Gradient Shimming System menu.

Gradient Shimming Files Menu

The Gradient Shimming Files menu is used for loading and copying shimmaps. To open this menu, click on Shimmap Files in the Gradient Shimming Map menu.

Button	*Description*
cd to Userdir or	Change directory to `userdir` shimmap.
cd to Systemdir	Change directory to `systemdir` shimmap.
Copy to Userdir or	Copy selected shimmap into user shimmap directory.
Copy to Systemdir	Copy selected shimmap into system shimmap directory.

Button	*Description*
Make Systemdir	Make system shimmaps directory if user is `vnmr1`.
Load Shimmap	Load files for selected shimmap.
Load Shimmap & Params	Load files and parameters for selected shimmap.
Rename	Rename selected shimmap under a new mapname.
Return	Return to the Gradient Shimming Map menu.

Gradient Shim Setting Menu

The Gradient Shim Setting menu sets shim values. To open this menu, click on Set Shims in the Gradient Shimming System menu.

Button	*Description*
Starting Shims	Set shims from when Gradient Shimming System menu was entered.
Old Shims	Set shims from before first iteration of gradient shimming.
New Shims	Set shims from last iteration of gradient shimming.
Min Shims	Set shims from minimum rms err in last set of gradient shimming iterations.
Return	Return to the Gradient Shimming System menu.

Gradient Shimming Display Menu

The Gradient Shimming Display menu is used for displaying items associated with gradient shimming. To open this menu, click on Display in the Gradient Shimming System menu.

Button	*Description*
dgs	Display shim parameters.
List Shims	Display current mapname and last shim changes.
Display Shimmap	Display current shimmap used by gradient shimming.
Display Fit	Display shim fit from last iteration of gradient shimming.
Show Record	Display record of shim adjustments from last gradient shimming run.
Plot	Enter Gradient Shimming Plot menu.
Return	Return to the Gradient Shimming System menu.

Gradient Shimming Plot Menu

The Gradient Shimming Plot menu is used for printing and plotting shim parameters and files. To open this menu, click on Plot in the Gradient Shimming Display menu.

Button	*Description*
Print dgs	Print shim parameters.
Print Shims	Print current mapname and last shim changes.
Plot Shimmap	Plot current shimmap.
Plot Fit	Plot last iteration shim fit.
Plot b0	Plot `b0` shim plot.
Return	Return to the Gradient Shimming Display menu.

Automated Shimming Menu

The Automated Shimming menu is used for running automated gradient shimming after a shimmap is made. To open this menu, click on Main Menu | Setup | Shim.

Button	*Description*
Lock Autoshim	Start lock autoshim using current `method`.
Lock Autoshim z1z2	Start lock autoshim on z1z2.
Gradient Autoshim on Z	Start gradient autoshim on z-axis shims
Quit Gradient Shim	End gradient shimming and return to previous experiment
Return	Return to Acquisition Parameter Setup menu.

Gradient Autoshimming Files Menu

The Gradient Autoshimming Files menu is used for loading shimmaps. To open this menu, enter `gmapshim('files')`.

Button	*Description*
cd to Userdir or	Change directory to `userdir` shimmaps.
cd to Systemdir	Change directory to `systemdir` shimmaps.
Current Mapname	Show current mapname used for gradient shimming.
Load Shimmap	Load files and parameters for selected shimmap.
Load Shimmap & Params	Load files and parameters for selected shimmap.
Return	Return to Main menu.

Chapter 7. Acquiring Data

Sections in this chapter:

- 7.1 “Setting Frequency-Related Parameters” this page
- 7.2 “Setting Pulse-Sequence-Related Parameters” page 185
- 7.3 “Creating and Editing Experiment Text Files” page 197
- 7.4 “Performing Acquisition” page 198
- 7.5 “Applying Digital Filtering” page 209

7.1 Setting Frequency-Related Parameters

With a spectrometer configured to perform the proper experiment, and a sample in place, spinning, locked, and shimmed, you are ready to select parameters to acquire data. There are two aspects to selecting parameters. The first is the frequency-related aspect—setting the position and size of the spectral window. The second is the pulse sequence-related aspect. The following section covers frequency-related parameters. Selecting pulse sequence-related parameters are described in “Setting Pulse-Sequence-Related Parameters” on page 185.

Frequency Setting

Table 24 lists frequency-related parameters and related commands.

Starting with VNMR version 4.3, the selection of frequencies for the observe channel and the decouplers is done differently from earlier versions of VNMR. The mechanism of setting frequencies is essentially the same; for example, entering `tn='H1'` selects the proton frequency. But in earlier versions, that resulted in `sfrq` being set to a value of the ^{1}H frequency taken from a nucleus table. When a data acquisition was requested with the `go` command, the value of `sfrq` was combined with information about the lock (`lockfreq`), solvent, and the small offset (`tof`) to generate the final frequency.

In the new scheme, when `tn='H1'` is entered, the ^{1}H frequency is again taken from the nucleus table, but then the `setfrq` command is called by the system. `setfrq` immediately combines the frequency from the table with information about the lock, solvent, and small offset and stores the result in the parameter `sfrq`. The result is that when a data acquisition is requested with `go`, no further adjustment of the value of `sfrq` is needed. In other words, the value of `sfrq` (and `dfrq`, `dfrq2`, `dfrq3`, `dfrq4` for decouplers) is the exact frequency that will be used. The benefits of the new approach are that the frequency is readily apparent and, more importantly, the calculation of ppm scales, which are based on the value of `sfrq`, are exact. Also, data that is stored can be recalled later on any system, and the correct frequency at which the data were obtained will be known—an essential part of good laboratory practice.

Table 24. Acquisition Frequency-Related Commands and Parameters

Commands	
`centersw`	Move cursor to center of spectrum
`minsw`	Reduce spectral width to minimum required
`movesw<(width)>`	Move spectral window according to cursors
`movetof<(frequency)>`	Move transmitter offset
`sd,sd2,sd3`	Set decoupler frequency to cursor position
`sda sd2a sd3a`	Set decoupler frequency array
`setfrq<(channel)>`	Set frequency of rf channels
`setsw(downfieldppm,upfieldppm)`	Set spectral width
Parameters	
`cr` {number}	Current cursor position
`delta` {number, in Hz}	Difference of two frequency cursors
`dfrq`, `dfrq2`, `dfrq3`, `dfrq4` {number, in MHz}	Transmitter frequency of decoupler
`dn`, `dn2`, `dn3`, `dn4` {string}	Nucleus of decoupler
`dof`, `dof2`, `dof3`, `dof4` {number, in Hz}	Frequency offset for decoupler
`lockfreq` {'n', 1 to 160, in MHz}	Lock frequency
`rfband` {string using 'h', 'l', 'c'}	RF band in use
`rfchannel` {string using '1', '2', '3', '4'}	Independent control of rf channel selection
`sfrq` {number, in MHz}	Transmitter frequency of observe nucleus
`solvent` {string in /vnmr/solvents}	Lock solvent
`sw` {number, in Hz}	Spectral width
`tn` {string in /vnmr/nuctables}	Nucleus for observe transmitter
`tof` {number, in Hz}	Frequency offset for observe transmitter

It is essential that `lockfreq` parameter for lock frequency be set correctly in order to observe NMR signals. On *MERCURY-VX*, *MERCURY*, UNITY*INOVA*, UNITY*plus* and *GEMINI 2000* systems, `lockfreq` must be set to the actual deuterium frequency. See the description of `lockfreq` in the *VNMR Command and Parameter Reference* for values. On UNITY and VXR-S 300-, 400-, and 500-MHz systems, the lock transmitter is equipped with a series of thumbwheel switches. These switches are used to adjust the lock frequency if the field drifts out of the range of the field offset control (the `z0` parameter). The starting value of these switches varies: 200-MHz systems typically start at 1.210, 300-MHz at 1.206; 400-MHz at 1.145, 500-MHz at 1.479, and 600-MHz at 153.845 (lock synthesizer). As the field decays, this number must be set downward to lower the lock frequency. Under normal, day-to-day operation, you will not need to change this value.

The `rfband` parameter (on all systems except *MERCURY-VX*, *MERCURY*, and *GEMINI 2000*) indicates the rf band in use for each channel: `'h'` indicates the high rf band for a channel, `'l'` indicates the low rf band, and `'c'` (for calculated) indicates that the system calculates the correct amplifier band, based on the selected frequency. The value of `rfband` is written as a string (e.g., `rfband='hlc'`) with the first channel determined by the first character, the second channel by the second character, etc.

The parameter `rfchannel` is available to give override capability over the selection of rf channels. Refer to the description of `rfchannel` in the *VNMR Command and Parameter Reference* for details.

Transmitter and Decoupler Positioning

The `movetof<(frequency)>` macro moves the transmitter offset parameter `tof` so that the current cursor position, defined by `cr`, becomes the center of the spectrum. If

referencing was used, `movetof` maintains the referencing. If you wish to specify the transmitter frequency directly, rather than using the cursor position, enter a value for the `frequency` argument. This provides a convenient method of moving the transmitter frequency outside the current spectral window.

The macro `sd` sets the first decoupler offset `dof` to place the first decoupler at the cursor position in the spectrum. Similarly, `sd2` sets `dof2`, and `sd3` sets `dof3`, for the second and third decouplers. These macros assume homonuclear operation—the decoupler nucleus (`dn`, `dn2`, or `dn3`) is the same as `tn`.

To set an array of decoupler offset values, use the macro `sda` for the first decoupler, the macro `sd2a` for the second decoupler, and the macro `sd3a` for the third decoupler. These macros also assume homonuclear operation.

Spectral Window

Spectral window size is adjusted with the spectral width parameter `sw` (see Figure 52). The spectral width determines the sampling rate for data, which occurs at a rate of `2*sw` points per second (actually `sw` complex points per second). The sampling rate itself is not entered, either directly or as its inverse (known on some systems as the “dwell time”).

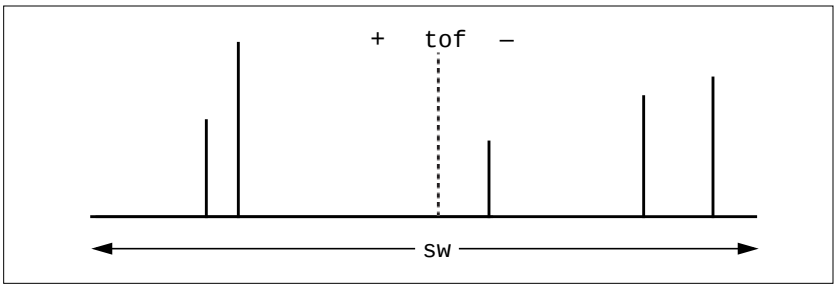


Figure 52. Positioning the Spectral Window

With two cursors displayed, the macro `movesw<(width)>` uses the parameters `cr` and `delta` to calculate a new spectral width sw and a new transmitter offset `tof`. If referencing was used, it is also adjusted. The macro also sets `sp` and `wp` to display the spectral window. Entering a `width` argument to specify the spectral width allows making an adjustment more precise than if based on the cursors.

The macro `setsw(downfieldppm,upfieldppm)` sets the parameters `sw` and `tof` for the given spectral window. `setsw` also does referencing.

The `centersw` macro moves the cursor to the center of the spectrum.

The `minsw` macro searches the spectrum for peaks, sets new limits accordingly, and then calls `movesw` to calculate a new transmitter offset `tof` and a new spectral width `sw`.

7.2 Setting Pulse-Sequence-Related Parameters

The second step in setting experimental parameters is the pulse sequence-related aspect. Table 25 lists pulse-sequence-related parameters and related commands and macros. Most experiments will be acquired using a pulse sequence known as the standard two-pulse, or S2PUL. The `s2pul` macro converts the current experiment to an experiment suitable for S2PUL. Figure 53 shows the parameters relevant to this pulse sequence and to many other pulse sequences. The pulse sequence name is stored in the parameter `seqfil`.

Table 25. Acquisition Pulse-Sequence-Related Commands and Parameters

Commands	
`dmfadj<(tipangle_resolution)>`	Adjust tip-angle resolution time for 1st decoupler
`dmf2adj<(tipangle_resolution)>`	Adjust tip-angle resolution time for 2nd decoupler
`dmf3adj<(tipangle_resolution)>`	Adjust tip-angle resolution time for 3rd decoupler
`dmf4adj<(tipangle_resolution)>`	Adjust tip-angle resolution time for 4th decoupler
`dps<(file)>`	Display pulse sequence
`ernst(t1_estimate<,90_pulse_width>)`	Calculate the Ernst angle pulse
`hoult`	Set `alfa` and `rof2` according to Hoult
`p1(flip_angle<,90_pulse_width>)`	Enter pulse width for `p1` in degrees
`pps<(file)>`	Plot pulse sequence
`pw<(flip_angle<,pulse_width>)`	Enter pulse width for pw in degrees
`s2pul`	Set up parameters for standard 2-pulse sequence
`time<(<hours,>minutes)>`	Display experiment time or recalculate nt
Parameters	
`alfa` {0 to 100000000, in ms}	Set alfa delay before acquisition
`at` {number, in seconds}	Acquisition time
`ct` {number, non-user enterable}	Completed transients
`d1` {number, in seconds}	First delay
`d2` {number, in seconds}	Second delay
`dhp` {'n',number}	Decoupler high power with class C amplifier
`dlp` {'n',number}	Decoupler low power with class C amplifier
`dm`, `dm2`, `dm3`, `dm4` {string}	Decoupler mode
`dmf`, `dmf2`, `dmf3`, `dmf4` {number, in Hz}	Decoupler modulation frequency
`dmm`, `dmm2`, `dmm3`,`dmm4` {string}	Decoupler modulation mode
`dpwr`, `dpwr2`, `dpwr3`, `dpwr4` {number,in dB}	Power level for decoupler with linear amplifier
`dpwrf`, `dpwrf2`, `dpwrf3` {number}	Decoupler fine power
`dpwrm`, `dpwrm2`, `dpwrm3` {number}	Decoupler linear modulator power
`dres`, `dres2`, `dres3`, `dres4` {number, in deg.}	Tip-angle resolution for WFG decoupling
`dseq`, `dseq2`, `dseq3` {string}	Decoupler sequence
`fb` {number,in Hz}	Filter bandwidth
`gradtype` {string}	Gradients for X, Y, and Z axes
`homo`, `homo2`, `homo3`, `homo4` {'y','n'}	Homodecoupling control for decoupler
`np` {number, constrained to multiple}	Number of data points
`nt` {number}	Number of transients
`p1` {number, in microseconds}	First pulse width
`pad` {number, in seconds}	Preacquisition delay
`pfgon` {'y 'or 'n' for each channel}	PFG amplifiers on/off control
`pw` {number, in ms}	Pulse width
`pw90` {number, in ms}	90-degree pulse width
`rof1` {number, in ms}	Receiver gating time preceding pulse
`rof2` {number, in ms}	Receiver gating time following pulse
`seqfil` {string}	Pulse sequence name
`ss` {'n',–32768 to 32767}	Steady-state pulses
`temp` {'n',number in celsius}	Sample temperature
`tpwr` {number, in dB}	Observe transmitter power level with linear amp.
`tpwrf` {0 to 4095, 4095 is max.}	Observe transmitter fine power
`tpwrm` {0 to 4095, 4095 is max.}	Observe transmitter linear modulator power
`vtc` {0 to 50, in celsius}	Variable temperature cutoff point

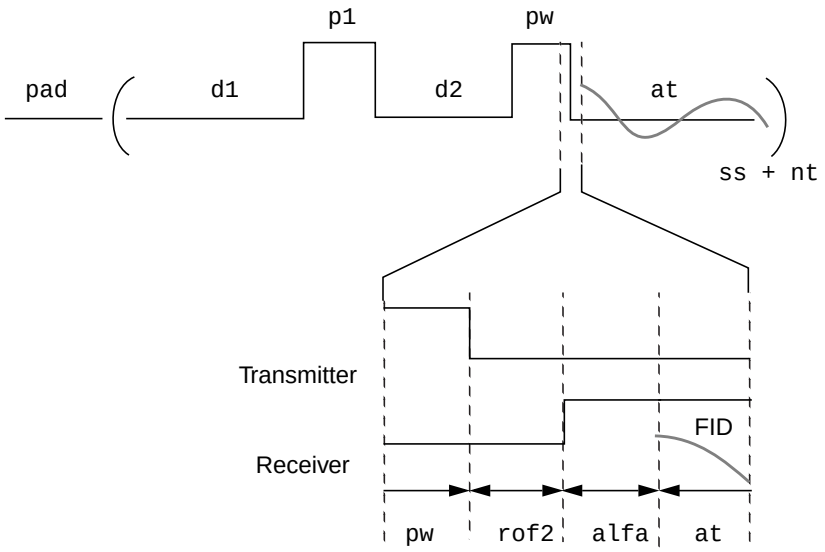


Figure 53. Acquisition Parameters for Standard Two-Pulse Sequence

Standard Two-Pulse Parameters

To allow the hardware to set up at the beginning of the experiment, the parameter `pad`, a preacquisition delay, is used. `pad` is usually set to 0.5 seconds. The other principal use of this parameter is for kinetics experiments.

The part of the experiment that is repeated is a sequence starting with a delay `d1`, then a pulse `p1`, followed by a delay `d2`, and another pulse `pw`. After dead times `rof2` (with receiver off) and `alfa` (with receiver on), `np` data points are acquired over a period of `at` seconds. This process is repeated `ss` + `nt` times, with the data actually acquired only during the `nt` number of transients and not during the first `ss` "steady-state" transients.

The `alfa` delay before acquisition consists of a variable part equal to the parameter `alfa` and a fixed part equal to `1/(beta*fb)`. The value of `beta` depends on the type of audio filter in the system and cannot be set by the user but is selected in `config` for the UNITY*INOVA*, UNITY*plus*, UNITY, and VXR-S systems. Because the total delay before acquisition is the sum of `alfa` and `1/(beta*fb)`, it is possible to shorten the delay beyond "normal" values by setting `alfa` negative. Refer to the description of `alfa` in the *VNMR Command and Parameter Reference* for the procedure.

`fb` is the filter bandwidth, in Hz, used to set the audio filters, which prevent noise of higher frequency than the spectral limits from "folding in" to the spectrum. The standard value of `fb` is 10% more than half of the spectral width `sw`. The `fb` parameter is automatically changed whenever the spectral width `sw` is changed, and thus is normally not a user-entered parameter. After `sw` has been change, `fb` may be changed to a different value.

The parameter `np` is generally calculated automatically when `sw` or `at` is changed. If a particular number of data points is desired, however, `np` can be entered, in which case `at` is calculated based on `sw` and `np`. Values of `at` that give a number of data points not a multiple of 2 (UNITY*INOVA*, UNITY*plus*, and UNITY systems) or 64 (*MERCURY-VX*, *MERCURY*, and GEMINI 2000 and VXR-S) will be readjusted automatically (actually depends on the output board, refer to the description of `at` in the *VNMR Command and Parameter Reference*).

ss is the number of complete executions of the pulse sequence not accompanied by data collection prior to the acquisition of the real data. In a multi-FID experiment, if ss is a positive value, the steady-state pulses are applied at the start of the first FID only; if ss is a negative value, the steady-state pulses are applied at the start of every FID.

nt is the number of transients to be acquired—the number of repetitions or "scans" performed to make up the experiment. To set up an indefinite acquisition, set nt to a very large number, (e.g., 1e9). The parameter ct (for "completed transients") is an informational parameter that changes during the course of an experiment to reflect the number of completed transients.

For "normal" 1D NMR, p1 and d2 are zero. The parameter d1 (used to allow recovery of magnetization back to equilibrium) is often zero as well, reducing the total pulse sequence to a pulse of pw µs followed by an acquisition time at, in seconds.

Before each pulse, the receiver is gated off for rof1 µs. rof1 is normally fixed as 10 µs. On systems where the amplifiers are normally "blanked" to give the best possible signal-to-noise, (i.e., they are turned off when the receiver is turned on), pulse sequences must be written so that the receiver is turned off for a sufficient time prior to a pulse to allow the amplifier to fully turn-on before the start of the pulse. Most pulse sequences are written so that this time is rof1.

On *INOVA* and *GEMINI 2000* systems, the receiver is off during the pulse sequence and on only during at. The amplifier can be unblanked at any time but no longer than 10 ms. Blanking and unblanking are implicitly done around pulses.

After the final pulse in each pulse sequence, the receiver is gated off for rof2 µs before the acquisition begins. If "pulse breakthrough" effects are seen (spike in the beginning of the FID), increasing rof2 can reduce or eliminate the problem.

The parameter pw90 stores the length of the 90° pulse, in µs. This parameter is not used by pulse sequences directly, but is used by a number of commands to assist in setting up special experiments. It is also used by certain output programs to be able to print the value of the pulse width in degrees instead of µs. Setting this parameter is the responsibility of the operator and is a function of the sample, probe, and system.

Commands for Setting Parameters

Given a desired flip angle in degrees, pw(flip_angle<,90_pulse_width>) calculates the flip time in µs and then enters the value into pw, (e.g., pw(45) enters a pw pulse of 45°). If the parameter pw90 exists and no second argument is entered, pw90 is taken as the 90° pulse. An entered second argument resets pw90. Similarly, the command p1(flip_angle<,90_pulse_width>) allows entry of the parameter p1 in degrees.

The command ernst(t1_estimate<,90_pulse_width>) uses an estimate of the T_1 time for a peak of interest and a 90° pulse width determined by the parameter pw90 to calculate the optimum ("Ernst") pulse width. The new pw is entered in the parameter table. If the parameter pw90 exists and no second argument is entered, pw90 is taken as the 90° pulse. Entering a value for the second argument resets pw90. The Ernst pw gives optimal sensitivity for the recycle time set by the user, as determined by d1 at at. More information about ernst can be found in R. R. Ernst and W. A. Anderson, *Rev. Sci. Inst.*, **37**, 93-102, (1966).

The setting of parameters alfa and rof2, the times that follow the final pulse, can be important where the flatness of the baseline is of concern. The hoult macro sets these values as described in D.I. Hoult, *J. Magn. Reson.* **51**:110 (1983).

The `time` macro estimates the acquisition time for the experiment, using the parameters `d1`, `d2`, `d3`, `mix`, `null`, `at`, `ni`, `sw1`, `ni2`, and `sw2` in the current experiment. By entering a requested time in the format `time(<hours>,minutes)`, the macro can recalculate `nt` so that the total acquisition time is approximately the requested time. Similarly, the `exptime` command estimates the experiment time for the current `seqfil`, using the parameters in the current experiment. `exptime` can also estimate the experiment time of a specified file (e.g., `exptime('s2pul')`).

The `dps` command reproduces a graphical display of the pulse sequence, complete with parameters as present in the `dg` display (see Figure 54).

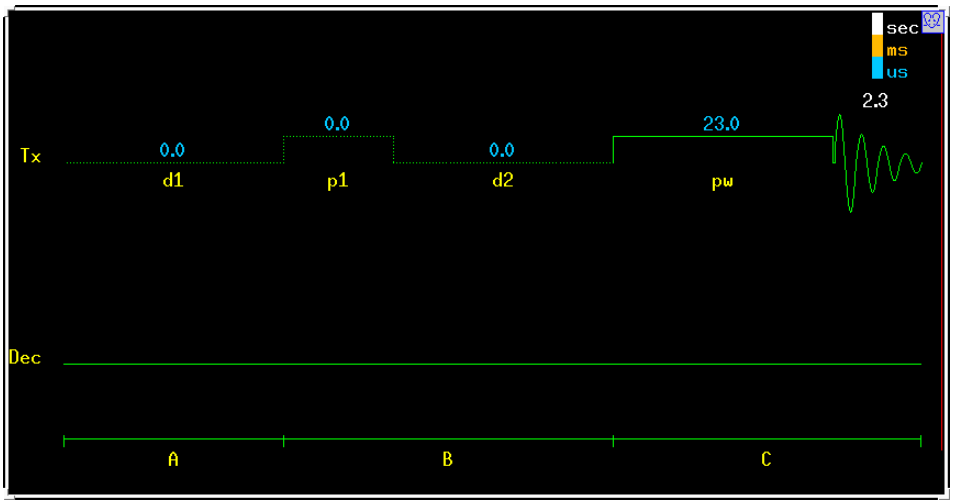


Figure 54. Graphical Pulse Sequence Display (`dps` Program)

This provides a quick and useful check of experimental conditions before beginning an experiment. `dps` also displays shaped pulses in which the height of the pulse reflects the power levels, spin lock, transmitter gating, observe transmitter power, and other information. The `pps` command plots the same display.

The button with the mouse face in the upper right corner opens the `dps` display control panel, shown in Figure 55. This panel provides control of how the pulse sequence is displayed, with timing, power or phase information, with or without parameter labels and values. When you click on a segment off a pulse sequence with the middle mouse button, the properties window displays information about that segment.

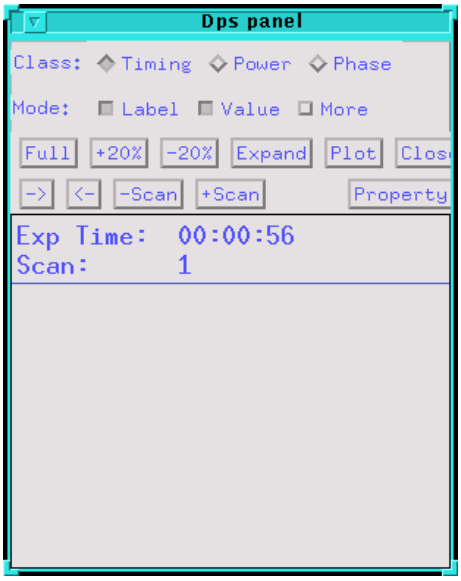


Figure 55. Display Properties Panel (`dps` Program)

The Property button opens a second window, shown in Figure 56, that allows you to set configuration options.

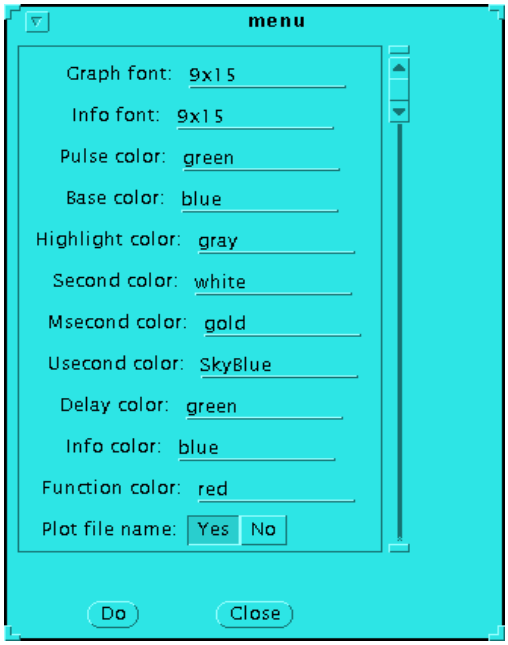


Figure 56. Property Button Window (`dps` Program)

The “Status” Concept

Every pulse sequence can be divided logically into “periods” of time. The standard two-pulse sequence, for example, can be divided as shown in Figure 57. This sequence has three logical periods, referred to in the diagram as A, B, and C. These periods are used in controlling the decoupler “status” (as well as the “homospoil” status, discussed later in this chapter).

For example, say we want the decoupler to be on during period A, on during period B, and off during period C. Using the letter `n` to signify “no” or an “off-status,” and `y` to signify “yes” or an “on-status,” we could then describe the desired decoupler status as `'yyn'`. Setting `dm='yyn'` will select this experiment, which in the heteronuclear case might produce a coupled spectrum with NOE, or in the homonuclear case might be used for solvent presaturation experiments. `dm='nny'` would give us an experiment with the decoupler only on during period C, the acquisition time, which in the heteronuclear case would be a decoupled spectrum without NOE.

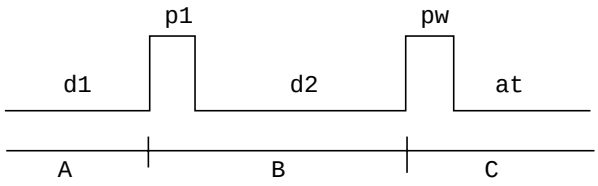


Figure 57. Logical Periods A, B, C in Standard Two-Pulse Sequence

Observe Transmitter and Decoupling Parameters

On all systems, transmitter power levels are set through attenuators, which are in turn controlled through a number of parameters. Figure 58 and Figure 59 show schematics for the attenuator configuration for different systems.

The parameter `tpwr` sets the observe transmitter power, which is under computer control on systems with linear amplifiers. `tpwr` can be given values from 0 to 63, or from –16 to 63, depending on the range of attenuators present in the system. In both cases, 63 is the maximum possible power.

The first decoupler mode parameter `dm` determines first decoupler output: if `dm='y'`, the first decoupler is on, and if `dm='n'`, the first decoupler is turned off. On UNITY*INOVA* and UNITY*plus* systems, setting `dm` to `'a'` or `'y'` specifies the asynchronous mode. In this mode, the decoupler rf is gated on and modulation is started at random places in the

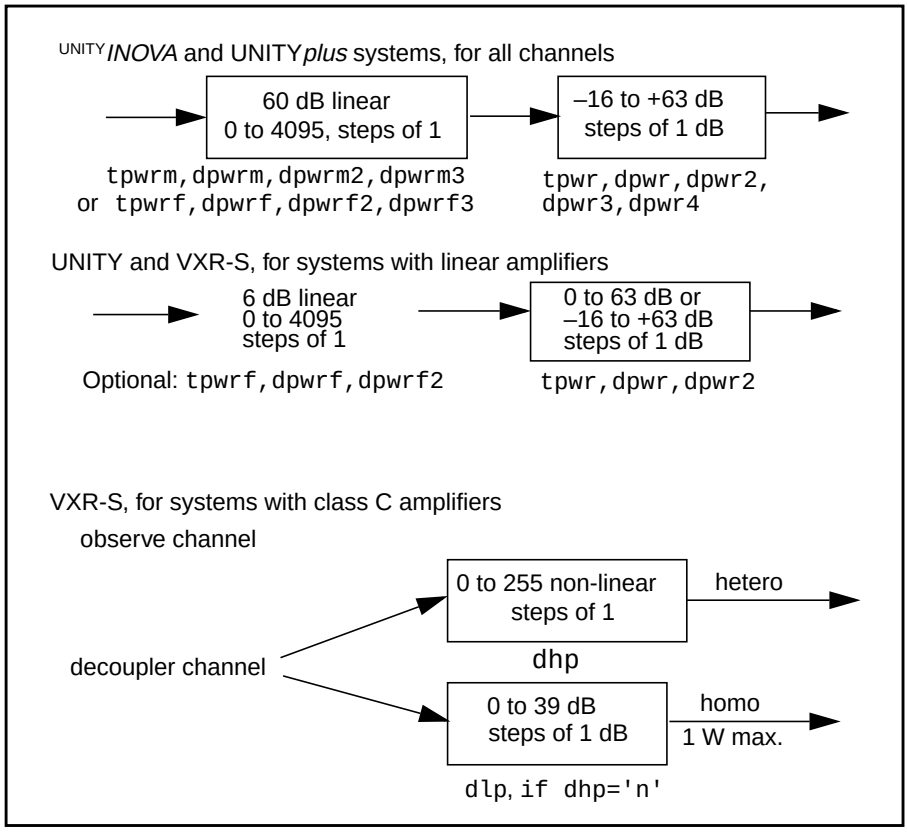


Figure 58. Attenuator Configurations (Part 1 of 2)

modulation sequence. Similarly, setting `dm` to `'s'` specifies the synchronous mode in which the decoupler rf is gated on and modulation is started at the beginning of the modulation sequence. The `'s'` and `'a'` values have meaning only on UNITY*INOVA* and UNITY*plus* systems. On UNITY and VXR-S systems, `'s'` and `'a'` are equivalent to `'y'`. The parameters `dm2`, `dm3`, and `dm4` function analogously to `dm`, except `dm2` works on the second decoupler, `dm3` on the third decoupler, and `dm4` on the fourth decoupler.

A UNITY*INOVA* or UNITY system is configured with transmitter fine power control. This fine power level is controlled by the `tpwrf` (or `tpwrm`) parameter. The attenuation is linear and spans 60 dB. A UNITY or VXR-S system can be optionally configured with fine power control. This fine power level is controlled by the `tpwrf` parameter. The attenuation is linear and spans 6 dB.

The parameter `homo` sets the homonuclear decoupling control for the first decoupler. On UNITY*INOVA* or UNITY*plus* systems, setting `homo` to `'y'` specifies that the receiver is gated, which is done by controlling the observe L.O. (local oscillator) line. The first decoupler rf, amplifier, and preamplifier are gated only if `dm ='y'`. If `dm='n'`, no gating of these signals takes place. When `homo='y'`, the parameter `dmm` should be set to `'c'` for continuous wave (CW) modulation. Setting `homo` to `'n'` specifies no gating.

On UNITY and VXR-S systems, setting `homo` to `'y'` selects time-shared decoupling, which is appropriate for homonuclear decoupling in which the receiver is gated off when the decoupler is on. Setting `homo` to `'n'` disables decoupler time-sharing, which is appropriate for heteronuclear decoupling or for cases in which the decoupler is off during acquisition.

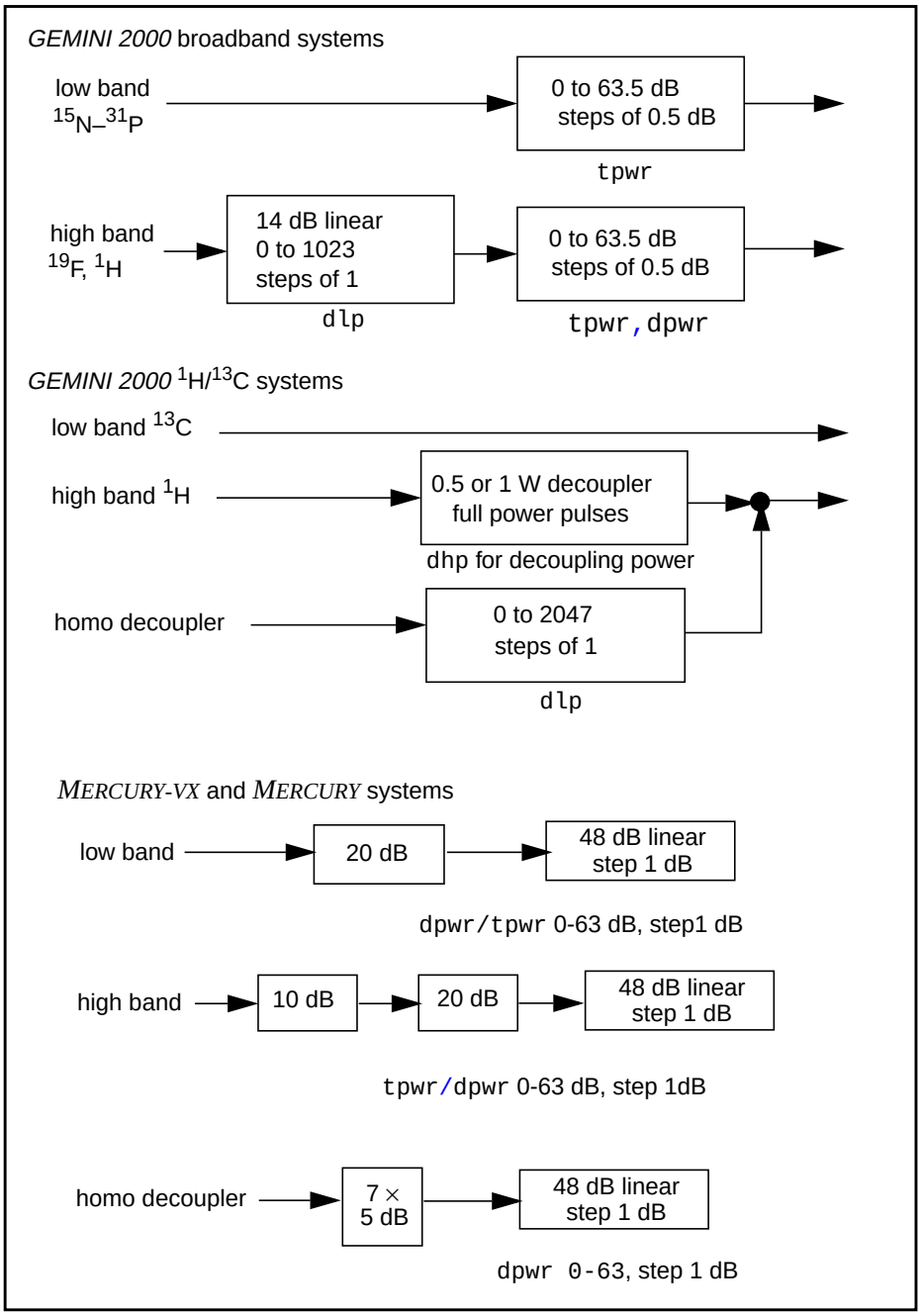


Figure 59. Attenuator Configurations (Part 2 of 2)

On UNITY systems and any system with a type 2 or 3 interface board (`apinterface=2` or `apinterface=3`), `homo` does not control any signal routing; the position of the relevant relays is controlled by whether homonuclear decoupling (`tn` equals `dn`) or heteronuclear decoupling (`tn` not equal to `dn`) is in effect. On systems with the type 1 interface board (`apinterface=1`), `homo='y'` also causes the decoupler signal to be combined with the observe signal before being sent to the probe.

On UNITY*INOVA* and UNITY*plus* systems only, the parameter `homo2` for the second decoupler, `homo3` for the third decoupler, and `homo4` for the deuterium decoupler channel

as the fourth decoupler are equivalent to the parameter homo. homo2 works in conjunction with the parameters dm2, dmm2, homo3 works with parameters dm3 and dmm3, and homo4 works with dm4 and dmm4.

On *MERCURY-VX*, *MERCURY*, and *GEMINI 2000*, homo has no meaning. Gated (homo) decoupling is used if the transmitter nucleus tn is ^{1}H or ^{19}F, and the decoupler mode dm is set to 'y'.

CAUTION: **Decoupler power greater than 2 watts in a switchable probe will damage the probe. Always carefully calibrate high-power decoupling to avoid exceeding 2 watts of power. The maximum value for dpwr on a 200-, 300-, or 400-MHz system with a linear amplifier on the decoupler channel has been set to 49, corresponding to approximately 2 watts of power. Before using dpwr=49 for continuous decoupling, ensure safe operation by measuring the output power. This safety maximum may be adjusted in the config program.**

On systems with class C amplifiers on the first decoupler channel, the parameter dhp controls the decoupler high-power level and the parameter dlp controls the low-power level, usually for homonuclear decoupling. dlp is only active if dhp='n'. dhp runs from 0 to 255 (maximum) in uncalibrated, non-linear units. Specific values of dhp should be calibrated periodically for any particular instrument and probe combination. dlp specifies dB of attenuation of the decoupler, below a nominal 1 watt value.

In addition, on *GEMINI 2000* broadband systems with fast switching attenuators, dlp controls a fine attenuator over 14 dB in 1023 steps in line with the coarse attenuator. For *GEMINI 2000* ^{1}H/^{13}C systems, dhp control the heteronuclear decoupler power: 0.5 or 1 watt. dlp controls the homodecoupler power: 0 to 2047.

On systems equipped with a linear amplifier on the first decoupler channel, the parameter dpwr sets the decoupler power, which is under computer control. dpwr can be given values from 0 to 63, or from –16 to 63, depending on the range of attenuators present in the system. In both cases, 63 is the absolute maximum power. However, the output power should be measured to make sure a maximum of 2 watts is applied to switchable probes. This safety maximum, which limits the value that can be entered for the parameter dpwr, can be adjusted in the config program. The parameters dpwr2, dpwr3, and dpwr4 set the decoupler power for the second, third, and fourth decoupler channels, respectively. These parameters can also have safety maximums adjusted in config. dhp and dlp are nonfunctional on *MERCURY-VX*, *MERCURY*, UNITY*INOVA*, UNITY*plus*, UNITY, and VXR-S systems with a linear amplifier on the decoupler channel.

If the system is configured with a fine attenuator on one or more of the decouplers, the decoupler fine power level is controlled by the dpwrf, dpwrf2, and dpwrf3 parameters for the first, second, and third decouplers, respectively. Decoupler fine attenuators are linear and span 60 dB on UNITY*INOVA* and UNITY*plus* systems, or 6 dB on UNITY and VXR-S systems.

UNITY*INOVA* and UNITY*plus* systems are configured with linear modulators on all transmitters. The linear modulator power of each transmitter is set by tpwrm, dpwrm, dpwrm2, and dpwrm3, or by tpwrf, dpwrf, dpwrf2, and dpwrf3.

Decoupler Modes

The dmf parameter controls the modulation of the first decoupler (dmf2 for the second decoupler, dmf3 for the third decoupler, and dmf4 for the fourth decoupler) using the (optional) WALTZ-16 decoupling. After calibrating the decoupler field strength γH_2, dmf

(or dmf2 to dmf4) should be set to equal 4*γH$_2$/2π or 1/pw90. In f (efficient) mode decoupling, dmf (and dmf2 to dmf4) is inactive on UNITY, but active on *MERCURY-VX*, *MERCURY*, UNITY*INOVA* and UNITY*plus* systems (see the *VNMR Command and Parameter Reference* for details). The macros dmfadj, dmf2adj, dmf3adj, and dmf4adj adjust the values of dmf, dmf2, dmf3, and dmf4, respectively, when using waveform generator programmable decoupling.

Starting with VNMR version 4.2, significant changes were made in the values for the parameter dmm, which sets the first decoupler modulation mode. Although dmm='c' still sets the decoupler to continuous or single-frequency decoupling, the values of dmm='s' and dmm='e' in previous versions of VNMR are no longer valid and, if used, generate an error message. Before VNMR version 4.2, dmm='s' could be used to set WALTZ-16 decoupling. This is no longer true: dmm='w' must be used to choose WALTZ-16 decoupling and dmm='f' must be used to choose fm-fm (efficient) decoupling.

Several other efficient decoupling schemes are available on *MERCURY-VX*, *MERCURY*, UNITY*INOVA*, and UNITY*plus* systems and are chosen with dmm: dmm='g' sets GARP decoupling, dmm='m' sets MLEV-16 decoupling, and dmm='x' sets XY32 decoupling. Refer to the description of dmm in the *VNMR Command and Parameter Reference* for other modulation modes available.

In the standard two-pulse sequence, dmm normally has just a single "state," since the decoupler modulation remains normally unchanged during the pulse sequence. Multiple states are possible; for example, dmm='ccw' gives single-frequency decoupling during the first part of the pulse sequence, and WALTZ-16 decoupling during acquisition. The parameters dmm2, dmm3, and dmm4 function the same for the second, third, and fourth decouplers, respectively, as dmm does for the first decoupler.

For systems with a waveform generator on a decoupling channel, set dmm to 'p' to select programmable decoupling using that waveform generator. To specify the decoupling sequence during any period of waveform generator programmable decoupling, use the dseq parameter for the first decoupler, dseq2 for the second decoupler, and dseq3 for the third decoupler. The parameters dres, dres2, dres3, and dres4 control the tip-angle resolution used within a programmable decoupling sequence on the first, second, third, and fourth decouplers, respectively. See the manual *VNMR User Programming* for further information on pulse control of waveform generators.

The following values are typical for decoupling on *MERCURY-VX*, *MERCURY*, UNITY*INOVA*, UNITY*plus*, UNITY, and VXR-S systems:

- Homonuclear decoupling with linear amplifiers:

dm='y'	Decoupler mode on
homo='y'	Homonuclear decoupling on
dmm='c'	Decoupler modulation mode is continuous wave
dpwr=5 to 15	Decoupler power level range (dlp, dhp nonfunctional)

- Heteronuclear decoupling with linear amplifiers:

dm='y'	Decoupler mode on
homo='n'	Homonuclear decoupling off
dmm='w'	WALTZ-16 decoupling
dpwr=40	Decoupler power level (dlp, dhp nonfunctional)
dmf=10000	Decoupler modulation frequency

- Homonuclear decoupling with class C amplifiers:

`dm='y'`	Decoupler mode on
`homo='y'`	Homonuclear decoupling on
`dmm='c'`	Decoupler modulation mode is continuous wave
`dhp='n'`	Decoupler high power off
`dlp=15` to `25`	Decoupler low power level range

- Heteronuclear decoupling with class C amplifier:

`dm='y'`	Decoupler mode on
`homo='n'`	Homonuclear decoupling off
`dmm='w'`	WALTZ-16 decoupling
`dhp=70`	Decoupler high power level
`dmf=9900`	Decoupler modulation frequency

The following values are typical for decoupling on *GEMINI 2000* systems:

- Homonuclear decoupling with linear amplifiers:

`dm='y'`	Decoupler mode on
`dmm='c'`	Decoupler modulation mode is continuous wave
`dpwr=6` to `20`	Decoupler power level range
`dlp=0` to `1023`	Fine attenuator control range

- Heteronuclear decoupling with linear amplifiers:

`dm='y'`	Decoupler mode on
`dmm='w'`	WALTZ-16 decoupling
`dpwr=45`	Decoupler power level
`dmf=10000`	Decoupler modulation frequency
`dlp=1023`	Fine attenuator control

- Homonuclear decoupling with class C amplifiers:

`dm='y'`	Decoupler mode on
`dlp=1500` to `2047`	Homodecoupler power level range

- Heteronuclear decoupling with class C amplifier:

`dm='y'`	Decoupler mode on
`dmm='w'`	WALTZ-16 decoupling
`dhp=0.5,1`	Decoupler high power level
`dmf=9900`	Decoupler modulation frequency

Temperature-Related Control

For systems equipped with the optional variable temperature controller, the `temp` command opens the Temperature Control window, shown in Figure 60.

The Temperature Control window can be used for the following purposes:

- Turn off temperature control.
- Set temperature control on at a specified temperature in degrees C.

- Enable temperature control from within an experiment using the `temp` parameter and the `su`, `go`, `ga`, or `au` commands and macros.
- Alternatively, turn off experiment control of the temperature and allow only the Temperature Control window, shown in Figure 60, (and the command `sethw`) to set the temperature.

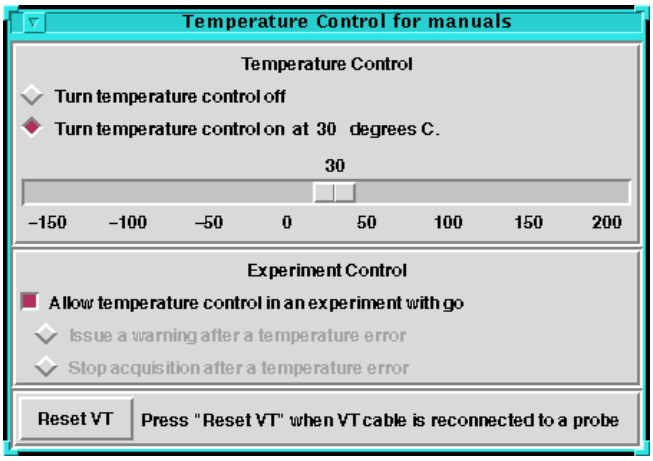

Temperature Control for manuals
Temperature Control
Turn temperature control off
Turn temperature control on at 30 degrees C.
30
−150 −100 −50 0 50 100 150 200
Experiment Control
Allow temperature control in an experiment with go
Issue a warning after a temperature error
Stop acquisition after a temperature error
Reset VT
Press "Reset VT" when VT cable is reconnected to a probe

Figure 60. Temperature Control Window

- Reset the temperature controller when the temperature cable is reconnected to a probe.

If the temperature is controlled only through the Temperature Control window, two actions (to be taken after a temperature error) can be selected:

- Display a warning but continue acquisition.
- Stop acquisition and display a warning.

If experiment control of temperature is selected, the two previous selections appear faded because they are inoperative, and the selection of the action to be taken after a temperature error is provided by the parameter `tin`.

Temperature-Related Parameters

For systems equipped with the optional variable temperature accessory, the `temp` parameter sets a sample's temperature between –150°C and +199°C. `temp='n'` disables the accessory. Another parameter, `vtc`, sets the temperature cutoff point. Above `vtc`, variable temperature gas flows straight into the probe, past the heater, and then past the sample. Below `vtc`, gas is routed first through the heat-exchange bucket (to be cooled by the heat-exchange fluid), then into the probe, and past the heater. `vtc` should be set depending on the temperature of the gas supply used for VT regulation.

For further information about temperature-related parameters, refer to the chapter on variable temperature operation in the manual *User Guide: Liquids NMR*.

Pulsed Field Gradient Related Parameters

For systems equipped with the optional Pulsed Field Gradient (PFG) module, the `pfgon` global parameter turns the PFG amplifier output on or off for the X, Y, and Z channels. For example, setting `pfgon='nnn'` tells PFG hardware to turn the amplifier off for all channels, and setting `pfgon='nny'` turns the amplifier output on for the Z channel only. A `su` or `go` command must be sent to activate `pfgon`. Another parameter, `gradtype`, tells the PFG hardware which channel is on.

For further information about PFG-related parameters, refer to the manual *User Guide: Liquids NMR*.

7.3 Creating and Editing Experiment Text Files

Each experiment has associated with it a file consisting of a block of text that describes the sample. Table 26 lists commands for working with experiment text files.

Table 26. Experiment Text File Commands

Commands	
`atext(string)`	Append string to the current experiment text file
`ctext`	Clear the text of the current experiment
`edit(file)`	Edit a file with user-selectable editor
`gettxt(file)`	Get a text file from a another file
`puttxt(file)`	Put a text file into another file
`text<(string)><:str_var>`	Display text or set new text for current experiment
`textvi`	Edit text file of current experiment

Creating and Editing a Text File

To enter text into the current experiment, use `text(text_string)`. For example, the command `text('24 Sep 1997')` places the following line of text into the file:

```
24 Sep 1997
```

To place more than one line of text in the text file, insert either a double backslash (`\\`) or a backslash `n` (`\n`) into the string to denote a new line. For example, entering the command `text('30% Menthol in CDCL3\\SW Probe\\24 Sep 1997')` sets the following three lines of text into the file:

```
30% Menthol in CDCL3
SW Probe
24 Sep 1997
```

To add a single line of text to the end of the current experiment text file, enter `atext(string)` (e.g., `atext('Series 10')`) appends this string to the text file:

```
Series 10
```

To use a text editor to edit the text file of the current experiment, enter `textvi`. The `textvi` macro lets you edit the text file from VNMR using the UNIX text editor `vi`. If you want to edit the file with a text editor other than `vi`, set the UNIX environmental variable `vnmreditor` to the name of the editor you want (e.g., `emacs`) and use the macro `edit(file)` instead of `textvi`. Refer to the description of `edit` in the manual *VNMR Command and Parameter Reference* for further information.

To clear or remove all the text presently in the text file of the current experiment, enter the `ctext` command.

Displaying and Handling a Text File

To display the text file in the current experiment, enter `text` without an argument.

To return text from a data file to the current experiment, use `gettxt(file)`, where `file` is the name of a VNMR data file. Text can be retrieved from a file on disk or from another experiment (e.g., `gettxt('vnmr/fiblib/fid1d')` gets file `fid1d`).

To save the text from the current experiment into a VNMR data file, use the command `puttxt(file)`. Text can be updated from a file on disk or from another experiment.

7.4 Performing Acquisition

Data are acquired through the macros `go`, `ga`, and `au`, through other macros containing `go`, `ga`, and `au`, or through the menu system (from the Main Menu, select the Acquire button). Table 27 lists acquisition-related command and parameters.

Initiating Acquisition

The main macros to initiate acquisition are `go`, `ga`, and `au`:

- `go` acquires the data and performs no processing. To run `go` from the menu system, select the Go button in the Acquire menu.
- `ga` automatically performs a weighted Fourier transformation after the FID has been collected. To run `ga` from the menu system, select the Go, Wft button in the Acquire menu.
- `au` allows for totally automatic and flexible data processing at a number of times during the experiment. To run `au` from the menu system, select the Automatic button in the Acquire menu.

Each of these macros initiates the acquisition of one or more FIDs, as determined by the acquisition parameters. `go`, `ga`, and `au` also perform several additional functions prior to starting data acquisition:

- Each macro executes two user-created macros if they exist. The first is `usergo`, a macro that allows the user to set up general conditions for the experiment. The second is a macro whose name is formed by `go_` followed by the name of the pulse sequence (from `seqfil`) to be used (e. g., `go_s2pul` or `go_dept`). This macro allows a user to set up experiment conditions suited to a particular sequence.
- If there is insufficient free disk space for the complete 1D or 2D FID data set to be acquired, `go` prompts the user with an appropriate message and aborts the acquisition initiation process. To override this function, enter `go('nocheck')`.
- On UNITY*INOVA*, UNITY*plus*, and UNITY, the pulse sequence language contains a power check for protecting the probe. For every timed event during a pulse sequence, the power levels of each rf channel are summed for each band (high band is ^{1}H, ^{19}F, or ^{2}H; low band is the remaining nuclei). Each band is associated with a coil in the probe. Limits for a coil cannot exceed a predefined safety limit.

  There are two common errors that often damage probes and related equipment. One is performing an rf pulse when the pulse width parameter is accidentally defined as a delay (in seconds) instead of a pulse (in microseconds). The second common error is to set the power level of the decouple at a high value for decoupler pulses and then forget to reset the power level to a lower level for CW decoupling. Both of these conditions can now be set to generate a warning and stop the experiment.

  Because probe protection could prevent performing certain experiments, the protection can be turned off temporarily by entering `go` with the `'nosafe'` keyword, (i.e., `go('nosafe')`). Turning off probe protection permanently can be done by setting the parameter `probe_protection` parameter to `'n'`.
- On UNITY*INOVA*, UNITY*plus*, UNITY, and VXR-S, the pulse sequence language contains a gradient level check for protecting the probe from gradients. This gradient checking is active for Performa II/III gradients and Performa XYZ gradients. For every timed event during a pulse sequence, the levels of each gradient are checked against predefined safety limits. The criteria are that a gradient may not be on at full power for more than 10 ms. There is also a 2% duty cycle limit. Finally, at the end of each FID accumulation, the duty cycle cannot exceed 50%.

Table 27. Commands and Parameters for Acquiring Data

Commands	
`aa`	Abort acquisition with error
`acqdisp(message)`	Display string on the acquisition status line
`acqmeter<('host')>`	Open the Acqmeter window
`acqstat<(remote_system)>`	Open the Acquisition Status window
`Acqstat <rem_sys> <-f file> <&>`	Open the Acquisition Status window (UNIX)
`au*`	Submit experiment to acquisition and process data
`autolist*`	Set up and start chained acquisition
`calcdim`	Calculate dimension of experiment
`errlog`	Display recent VNMR error messages
`expactive<(exp_number)><:ans>`	Determine if experiment has active acquisition
`explog`	Display log file of experiment
`ga<('nocheck')>`	Submit experiment to acquisition and FT the result
`gmapshim_au`	Start acquisition with gradient shimming
`go*`	Submit experiment to acquisition
`go_sequence`	Pulse sequence setup macro called by go, ga, and au
`halt`	Abort acquisition with no error
`jexp1, jexp2,...,jexp9`	Join existing experiment
`noise*`	Measure noise level of FID
`ra`	Resume acquisition stopped with sa command
`react<('wait')>`	Recover from error during werr processing
`sa<(option|number)>`	Stop acquisition
`showstat<(remote_system)>`	Display information about acquisition status (VNMR)
`showstat <remote_system>`	Display information about acquisition status (UNIX)
`unlock(exp_number)`	Remove inactive lock and join experiment
`usergo`	Experiment setup macro called by go, ga, and au
`wbs(string)`	Specify action when bs transients accumulate
`werr(string)`	Specify action when error occurs
`wexp(string)`	Specify action when experiment completes
`wnt(string)`	Specify action when `nt` transients accumulate
`* au<(<'nocheck'><,><'next'><,><'wait'>)>`	
`autolist(<option,>experiment1<,experiment2<,experiment3,...>)`	
`go<(<'acqi'><,'nocheck'><,'nosafe'><,'next'><,'sync'><,'wait'>)>`	
`noise<(excess_noise<,last_noise<,block_number>>)>:r1,r2,r3,r4,r5,r6`	
Parameters	
`acqstatus` {code number}	Acquisition status
`arraydim` {number}	Dimension of experiment
`bs` {1–32767 transients,'n'}	Block size
`celem` {number}	Completed FID elements
`date` {string}	Date (from UNIX system)
`dp` {'y','n'}	Double precision
`errloglen` {number}	Number of lines in VNMR error message display
`gain` {'n', number in dB}	Receiver gain
`hs` {y or n for each period}	Homospoil pulses
`hst` {number, in milliseconds}	Homospoil time
`probe_protection` {'n','y'}	Probe protection control
`wbs` {string}	When block size
`werr` {string}	When error
`wexp` {string}	When experiment completes
`wnt` {string}	When number of transients

- Whenever data are acquired, the current date is copied from the UNIX-level calendar and written into the acquisition parameters, thus maintaining a record of the date of acquisition. The `date` parameter contains the date that is copied.

To calculate the dimension of an experiment, enter the `calcdim` command. The result is put into the `arraydim` parameter. If an experiment is arrayed, `arraydim` is the product of the size of the arrays.

The `celem` parameter indicates the number of completed FIDs in an experiment. When `go` or `au` is entered, `celem` is set to 0. As each FID acquisition is completed, `celem` is updated. This parameter is most useful in conjunction with `wbs`, `wnt`, `wexp`, and `werr` processing macros (see Automatic Processing on page 191).

Shimming During an Acquisition

On UNITY*INOVA* systems only, you can use the Acquisition window to shim on your sample while an acquisition is in progress. The procedure is as follows:

1. If the Acquisition window is not open, enter `acqi` to open the window, shown in Figure 61.
2. Enter `su`, `go`, or `au` to start an acquisition.

   If you have connected `acqi` to the console and start an acquisition, `acqi` is disconnected. You can connect to `acqi` while acquisition proceeds.
3. To shim during the acquisition, click on the SHIM button.

   The shim panel appears so you can perform shimming as usual.

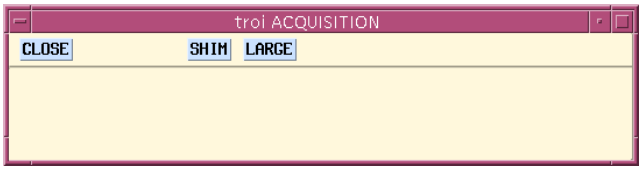


Figure 61. Acquisition Window (`acqi` Program)

The following features are not accessible from the SHIM window (shown in Figure 62) during acquisition:

- The z0/pwr/gn/ph panel that lets you access the lock system from the shim panel.
- The autoshim panel.
- The lock gain slider adjustment

You must use the same account that was used to start the acquisition. Therefore, if `vnmr1` starts an acquisition, only the acquisition process running as `vnmr1` can connect to the console while the acquisition remains active. If you log in as `vnmr1` to the spectrometer on your X display terminal, you can start `acqi` and it will connect to the console from the X display terminal.

Queueing Acquisitions

Under many circumstances, it is desirable to have the spectrometer perform more than one experiment on a single sample. Each time you enter `go`, `ga`, or `au`, the system first determines if an experiment is currently active. If not, the experiment you are submitting becomes active; otherwise, the new experiment is “queued,” and waits for the current experiment (and other previously queued experiments) to complete before starting. Note that you cannot queue acquisition commands (`go`, `au`, etc.) from the same experiment directory (e.g., `exp1`), but multiple `shim` commands can be queued.

To move an experiment to the head of the queue of experiments to be submitted to the acquisition system, enter the `go('next')` command. This command also has the effect of synchronizing VNMR command execution with the submission of experiments to the acquisition system. To accomplish this synchronization without putting the experiment at the head of the queue, enter the `go('sync')` command.

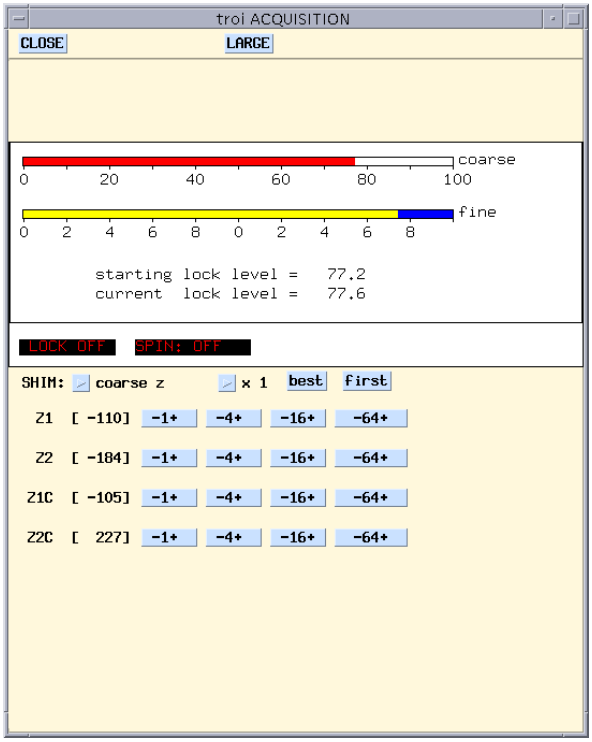


Figure 62. SHIM Window During Acquisition (`acqi` Program)

Experiments do not need to all be submitted at the same time. If you have started an experiment in `exp1`, for example, you might wait until that experiment is partially done and then, using those partial results, set up a follow-on experiment (perhaps a decoupling experiment) in `exp2`. Later, when `exp1` has completed and `exp2` is active, you could set up a third experiment, and use `exp3` to set up and submit it.

When an experiment is active, on all systems except the UNITY*INOVA*, you cannot use the Acquisition window to shim, and the `su` command (which is used to set up the spectrometer hardware for temperature changes, probe tuning, etc.) is irrelevant, but would be queued if started from another experiment. On UNITY*INOVA systems, you can shim on your sample while an acquisition is in progress* (see “Shimming During an Acquisition” on page 200).

Chained Acquisition

The `autolist` macro sets up parameters for chained experiments by executing the experiments given as arguments and then starting a chained acquisition, for example, `autolist('h1','c13','dept')`. The macro `au` is executed as part of `autolist` and should not be included in the arguments to `autolist`.

To start a new experiment based on the results of another experiment, use the `wexp` parameter.

To prevent another queued experiment from being started between two experiments, use the `'wait'` argument with the macros `go`, `ga`, and `au`. `'wait'` specifies that no acquisition will be started until `wexp` processing of an experiment is finished.

Use the `'next'` argument to change the processing order of experiments. `'next'` puts an experiment next in line (to the front of the queue) for acquisition. `'next'` is most useful for chained acquisitions and in automation.

If a third experiment is to be started based on the results of the first or second experiment, use both the `'wait'` and `'next'` arguments with `au`.

The `resume` command re-enables experiments to be submitted to the acquisition system, even if the `wexp` processing of an experiment that was started with `au('wait')` is not yet finished. `resume` can be useful if the processing macro extracts enough information to start the next experiment, identified by `au('next')`, but still has more processing to do.

Stopping and Resuming Acquisition

An experiment that has been submitted for acquisition can be stopped with the `sa` command. If the experiment is waiting for execution, no action is taken. If the experiment is active, it is stopped and data is retained. Options are available for stopping the experiment at several user-specified places during acquisition (only the first option is supported by *MERCURY* and *GEMINI 2000* systems):

- At the end of the next data accumulation (`ct`), e.g., `sa` or `sa('ct')`.
- At a multiple of the value of `ct`—can be used to complete a phase cycle before stopping, e.g., `sa(4)`.
- At the end of the next block size, e.g., `sa('bs')`.
- At the end of the next complete FID, e.g., `sa('nt')`.
- At the end of the next complete interleave cycle, i.e. the latest block size has been complete for all FIDs in the interleave cycle, e.g., `sa('il')`.

The command `ra` resumes an acquisition stopped with `sa`.

When experiments are queued, the behavior of `sa` and `ra` is more complex. If an experiment is active in `exp1` and queued in `exp2`, entering `sa` from `exp1` stops that experiment and immediately begins acquisition on `exp2`. Entering `sa` from `exp2`, on the other hand, removes `exp2` from the queue, without affecting the active experiment 1. Entering `sa` from an experiment that is neither active nor queued has no effect.

Entering `ra` likewise applies to the experiment from which it is entered. If `exp1` was stopped with `sa`, you must be joined to `exp1` to resume that acquisition with `ra`. If both `exp1` and `exp2` were stopped with `sa`, you can resume either one (or both), depending on whether you are joined to `exp1` or `exp2` when you enter `ra`. Note also that experiments resumed with `ra` go to the “end of the queue” if other experiments have started in the meantime.

Pausing, Halting, and Aborting Acquisition

Once an acquisition is in progress, it generally continues to completion; however, several situations can stop acquisition early. The system may detect an error, it may detect an overflow, or the operator may stop the system with an `aa` or an `sa` command.

The UNITY*INOVA* system (only) detects data overflow at 16 bits for `dp='n'` and 32 bits for `dp='y'` and responds with an error message

```
MAX. TRANSIENTS ACCUMULATED
```

Except under unusual circumstances, `dp='y'` should be used at all times (see also the section “Data Precision and Overflow” below). Overflowing `dp='y'` with real-time DSP (`dsp='r'`) is possible with greater than 4000 transients.

Another alternative, if `dp='n'`, is to change the maximum scaling constant `mxconst` to add additional scaling (refer to the *VNMR Command and Parameter Reference* for details, including a caution, about using `mxconst`).

If an acquisition is to be prematurely terminated (because sufficient signal-to-noise has been obtained or because the experiment has proved useless), the `aa` command to abort acquisition should be used (or the Abort Acq button on the Permanent Menu). If the experiment is active, it is aborted immediately, all data is discarded, and the experiment is interpreted as an error. Any data collected from an earlier block size transfer is retained. If any `werr` processing is defined, that processing occurs, followed by any queued experiments. The login name, and the FID directory path in `file` are used as keys to find the proper experiment to abort.

At times, it is convenient to abort an acquisition but have `wexp` processing occur instead of `werr` processing. The `halt` command is provided for this purpose. See the next section, "Automatic Processing," for more details on `wexp` and `werr` processing.

Under some circumstances, there is a delay between the time `go` is entered and the acquisition is started. During this time, instructions based on the selected pulse sequence are being generated. This is signified by the letters "`PSG`" appearing in the upper left corner of the status window. An `aa` or `halt` command issued under these circumstances reports that no acquisition is active but it instead stops the instruction generation process and the message "`PSG aborted`" appears.

Use `aa` or `halt` only if the data is not to be used or if a block size storage has taken place so that the data at the time of the last block is present; otherwise, the data is irretrievably lost.

Data Precision and Overflow

Single precision (16 bit, `dp='n'`) is mainly designed for a single application related to imaging. Because DSP (digital signal processing) can give you 20 bits of data in a single acquisition, the 16-bit data size is usually not desirable. The console will detect a numeric overflow in hardware and post an error. Even without DSP, the standard 16-bit ADC boards can theoretically overflow after one transient. Therefore, `dp='y'` is the preferred setting.

Overflowing `dp='y'` with `dsp='r'` (real-time DSP) is possible with greater than 4000 transients. Hardware DSP scales to 16 bits with `dp='n'` so that it will not overflow. As a result, many of advantages of hardware DSP are discarded.

Under some conditions, `dp='n'` is useful. The main example is "flash" imaging, where only one transient is typically taken, using very large data sets under fast conditions. In these experiments, the DTM memory (data-to-memory board memory, typically 16 Mbytes) can be filled up with rapidly acquired single-shot acquisitions. The `dp='n'` mode doubles the capacity of the DTM memory, increasing the number of increments in the experiment. If a cancellation experiment is carefully designed to avoid overflowing 16 bits, the `dp='n'` mode can cut the storage data size by a factor of 2. No down scaling is performed on UNITY*INOVA* so that the full available signal is always used. This use requires care in the cancellation cycle and an estimate when averaging will overflow 16 bits, so that `dp='y'` is still preferable for robust operation.

Automatic Processing

To examine data from the experiment in progress, the parameter `bs` and the concept of the "block-size" is provided. The data system uses two independent computers, the host computer and the acquisition computer. When the parameter `bs` is set to some number, say 64, the acquisition computer is instructed, after every 64 transients, to provide the accumulated data up to that point to the host computer to be stored in an appropriate disk file (overwriting earlier data). Thus, every `bs` transients, an updated version of the

experiment in progress is available for viewing by the user, who is communicating with the host computer. Typing `wft` (see Chapter 8, “Data Processing,” for weight and Fourier transform) processes the current FID as of the last `bs` transients and display the resulting spectrum on the screen.

This process can be made automatic, because the host computer can detect whenever new data is present on the disk, using the parameter `wbs`, which means “when block size.” If you set `wbs='wft'` and then type `au` (or use the Go, Periodic Wft button in the Acquire Menu), you are telling the computer “When block size (that is, when `bs` transients are completed), perform the action `wft`.” Now every 64 (or whatever the value of `bs` is) transients, the FID is automatically transformed and the spectrum displayed on the screen. Any command or macro can in fact be invoked to occur automatically (e. g., `wbs='dfid'`) display the FID after every `bs` transients. If acquisition is started by `go` or `ga`, `wbs` processing may still be set by using the `wbs` command, (e.g., `wbs('wft')`). `wbs` processing may also be disabled by entering `wbs('stop')`. Setting `bs='n'` before starting the acquisition disables this block-size storage. *If bs='n', data are stored on disk only at the end of the experiment, and. if the experiment is aborted prior to termination, data will be lost.*

There are other times when automatic processing is desirable:

- When an FID is finished, frequently you want it to be automatically transformed. You can accomplish this with the `wnt` (for “when number of transients”) parameter, (e.g., `wnt='wft'`). This particular action, in fact, is automatically performed by the `ga` command, since it is so common.
- When more than one FID is being accumulated, we may want to reserve one particular action to occur at the end of all of the FIDs. We might be performing a 2D experiment and, after all the data have been accumulated, we want to perform a 2D transform (for multidimensional NMR, see the manual *User Guide: Liquids NMR*). For this we use the `wexp` (for “when experiment”) parameter, (e.g., `wexp='wft2d'`).
- When an acquisition error occurs, some corrective action may be desirable. You can accomplish this with the `werr` (when error) parameter, (e.g., `werr='react'`).

Analogous to `wbs`, the commands `wnt` and `wexp` permit setting these automatic functions, even after `go` or `ga`, or to reset functions specified by the parameter `wbs`, `wnt`, and `wexp` and the `au` command.

Acquisition Status Window

The Acquisition Status window normally appears automatically on the screen when VNMR is started. If this window does not appear, or if it has been exited, start it by entering `acqstat` or by selecting Acquisition Status from the Workspace menu.

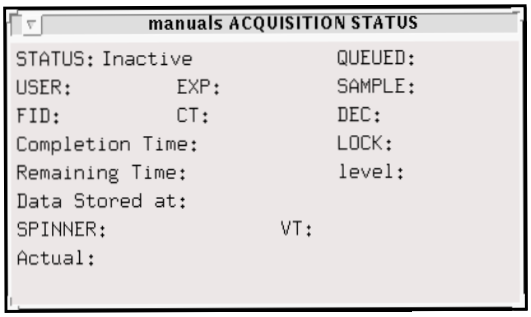


Figure 63. Acquisition Status Window (`acqstat` Program)

Figure 63 shows a typical Acquisition Status window when first opened. The display can contain 19 fields of acquisition status information, but all fields are not always displayed due to the hardware configuration of the system or the parameters set on the system.

Table 28 lists the possible fields, with a description of each field.

Table 28. Fields in the Acquisition Status Window (acqstat Program)

Field	*Description*
STATUS	Present status of acquisition The values displayed should be self-explanatory (e. g., “Shimming”) with two exceptions: “Active” means that the acquisition computer started but the console is not active yet, and “Inactive” means that `acqstat` cannot communicate with the acquisition computer or that the acquisition computer is not executing.
QUEUED	Number of experiments queued by multiple `go` commands
USER	Login name for owner of the experiment that is active
EXP	Number of the active experiment (e. g., `exp1`, `exp2`, `exp3`).
FID	Number of the FID being acquired if in an arrayed experiment
CT	Number of completed transients
DEC	Decoupler state: On, Off, Gated
SAMPLE	Sample number in magnet if in automation mode
LOCK	Lock status: Off, Regulated, Not Regulated
level	Present lock level
Completion Time	Estimated time when experiment will complete
Remaining Time	Remaining time (h,m,s) until the experiment completes
Data Stored at	Last time that data was transferred to disk.
SPINNER	Spinner status: Off, Regulated, Not Regulated
Actual	Actual spinner speed
Setting	Requested spinner speed
VT	Variable temperature unit status: Off, Regulated, or Not Regulated (if VT is set as present and `vttype=2`)
Actual	Actual temperature (if VT is set as present and `vttype=2`)
Setting	Requested temperature (if VT is set as present and `vttype=2`)

The look of the Acquisition Status window can be changed using the Acqstatus Setup window, which is shown in Figure 64. Open this window by clicking the right mouse button anywhere inside the Acquisition Status window and selecting Properties.

To quit the Acquisition Status window, click on the horizontal bar at the top of the window with the right mouse button and select Quit from the popup menu. Alternatively, to close the window to an icon, click on the inverted triangle in the upper left of the window with the left mouse button. When you want to view the acquisition status window again, reopen the window by double clicking the icon with the left mouse button.

Receiver Gain

Low gain in multiline, high-dynamic range samples can cause a number of problems, including intermodulation distortions, lower sensitivity, and extra lines in the spectrum. Too high a gain, on the other hand, can cause receiver overload and consequent baseline distortion. Autogain capability allows the observe channel to be set optimally for detecting and digitizing NMR signals from a wide variety of samples.

The parameter `gain` sets receiver gain, with `gain=60` representing the highest possible actual receiver gain and `gain=0` the lowest. (On *MERCURY-VX* and *MERCURY* systems, gain range is 0 to 38 dB; step size for gain is 2 dB. On *GEMINI 2000* systems, the highest receiver gain is `gain=40`. On UNITY*INOVA* and UNITY*plus* 500-, 600-, and 750-MHz systems only, the controllable usable range of `gain` is 18 to 60 when using low-band observe nuclei.) `gain` increases in steps of 2 dB. `gain='n'` activates Autogain, in which the gain is automatically adjusted at the start of acquisition for an optimum value. After the acquisition is finished, setting `gain='y'` then allows the value of `gain` to be read by typing `gain` followed by a question mark (i. e., `gain?`).

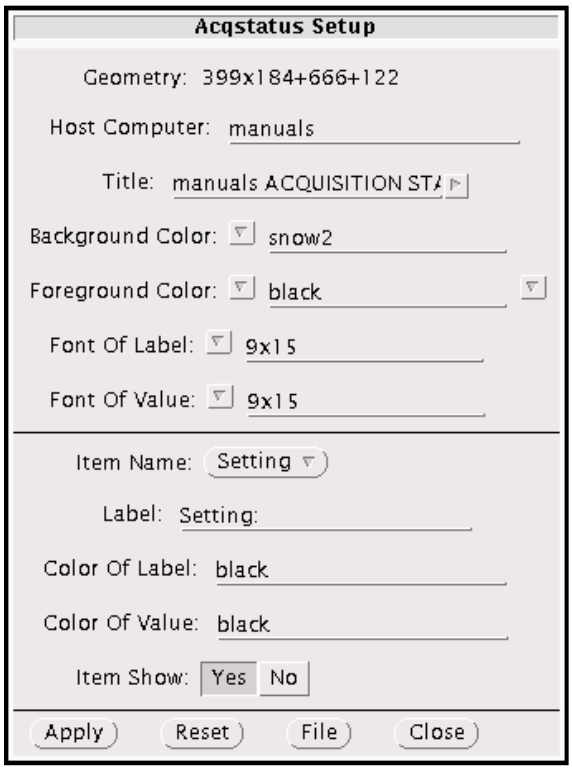


Figure 64. Acqstatus Setup Window (`Acqstatus` Program)

Homospoil

Homospoil is a process by which the homogeneity is temporarily made very bad ("spoiled") to cause any transverse magnetizations present at that time to decay rapidly to zero. The parameter `hs` turns on homospoil pulses at various times in some pulse sequences. If homospoil is activated by the `hs` parameter, (e.g., `hs='yn'`), the duration of the gradient pulse is controlled by the parameter `hst`.

GEMINI 2000 systems do not have homospoil so `hs` must be `'nn'`; otherwise, a warning message is displayed at a `go`, `ga`, or `au` command. `hst` is ignored on the *GEMINI 2000*.

File Protection

Two different processes (two different users or one user doing two different things simultaneously) should not access the same experiment at the same time. To prevent this simultaneous access, VNMR has an experiment lock system. The primary lock is a file in the user's VNMR directory named `lock_N.primary`, where `N` is the experiment number, 1 to 9. The directory contains the lock mode, the host name, and the ID of the process which has a lock on that experiment. The lock mode is a small number that distinguishes between foreground, background, and acquisition processing.

Since there is a possibility of a collision between two processes if each finds the experiment available and each attempts to access it at the same time, each process must first obtain a secondary lock, creating a file named `lock_N.secondary`. This file can only be created once, so it enforces a sequential access on the primary lock system. Since it is only accessed briefly and is deleted once the access is complete, you never see this file present under normal circumstances.

To override this protection system on an experiment, enter the command
`unlock(exp_number)`

where `exp_number` is the number of the experiment (e. g., `unlock(3)`). Use `unlock` only if you know the primary lock on the experiment is stale; that is, the process that has a lock on the experiment no longer exists. Should `unlock` not work, you can enter this command from VNMR as a workaround:
`shell('rm -f', userdir+'lock_n.primary')`

where `n` is the number of the experiment. In entering the `shell` command, do not use a wildcard character (such as a question mark or an asterisk) for the experiment. You should also not build this command into a macro because this would defeat experiment locking completely. There are definitely many instances in which a lock file exists for good reasons.

Remote Acquisition

Beginning with VnmrS version 4.1, control of acquisition is possible from a remote computer, terminal, or terminal emulator. Use of VNMR software from these devices is discussed in the manual *System Administration* and the user is referred there for further information on operation of VNMR itself remotely.

All data acquisition commands are supported. The only acquisition-related feature missing from remote operation with a terminal is the Abort Acq button, because the row of buttons containing that button is missing from the terminal environment. The equivalent keyboard command `aa` is functional. Prior to the release of VnmrX 4.3, remote interactive shimming using `acqi` was not supported, although remote computer shimming could be accomplished by using the parameters `wshim` and `method` as part of a `go`. Remote interactive shimming using `acqi` is fully supported in VnmrX 4.3 and later.

From a remote Sun computer, you can use the remote `Acqstat` command, which was described above. From terminals or non-Sun computers, access to the experiment status is provided with the `showstat` command. This command gives the same information as the Acqstat window but in a non-graphical manner. Other options include entering the command `explog`. Or you can enter the somewhat equivalent, but possibly preferable, command `shell('cat '+curexp+'/acqfil/log')` to show the complete file or `shell('tail +curexp+'/acqfil/log')` to show the tail or end of the log file. Either of the last two commands display in the text window the contents of the experiment log file, which shows when the experiment was submitted, when it was started, and (if done) when it is done.

During the course of the acquisition, block size complete messages and FID complete messages (and error messages, if present) will be reported. The value of ct also will be updated at the normal times. For all experiments, the parameters `wbs`, `wnt`, and `wexp` (and associated commands `wbs`, `wnt`, and `wexp`) are active, just as they are if acquisition is run locally.

The issue of multiple users arises. If an acquisition was initiated on the spectrometer by a user, say, "`vnmr1`," someone logging in remotely must also be "`vnmr1`" in order to stop that acquisition. If no acquisition is in progress, any user can initiate an acquisition remotely. No "remote lockout" is provided.

With a single user, the second issue that arises is shared use of an experiment. If you are "in," say, experiment 3 (`exp3`) when you leave the spectrometer, you will not be able remotely to join `exp3` when you log on from a remote terminal, because that experiment is "locked." If that is the experiment in which acquisition is progressing, you will be unable to affect that acquisition. The preferable solution to this problem is to use the `jexp`

command (e. g., `jexp2`) at the time you leave the spectrometer to join an experiment in which acquisition is neither proceeding nor queued.

If you forget to do this, there is a less desirable solution that can be executed remotely:

1. From UNIX, enter `ps -ef`.

   Listed are the "processes" that are running, with the "process number" shown in the first column of the listing.

2. Look for the process that begins `Vnmr –mforeground...`, and note the process number belonging to that process.

3. Enter `kill -3` #, where # is the process number from the previous step.

   The `kill -3` command causes the version of VNMR running on the spectrometer to act as if someone sitting there had typed `exit`; that is, in an orderly fashion it saves all its data and parameters and then exits (`kill -9`, which is more common, does not do this and is not the proper procedure).

4. After the spectrometer version of VNMR has exited, you can start VNMR from your terminal and enter any experiment you choose.

If the lock is inactive, the `unlock(exp_number)` command removes the lock from the specified experiment and joins the experiment. Note that `unlock` fails if the lock is still active or if the lock was placed on the experiment by the remote host.

Acquisition Information

Information about acquisition is saved at several locations:

- If `Acqproc` is active, the UNIX command `Acqstat` displays the current state of the acquisition process.
- An ASCII log file of acquisition activity in `/vnmr/acqqueue/MasterLog`. This file is not available on UNITY*INOVA* systems.
- An ASCII log file is also kept in `~user/vnmrsys/expn/acqfil/log` for acquisitions and in `~user/vnmrsys/expn/acqfil/sulog` for experiment setup.

Each of these log files will reset themselves to empty at 100 Kbytes so that the entire disk structure is not log-jammed.

The `expactive` command determines if the current experiment has an active acquisition. The results are displayed on line 3.

Acquisition Status Codes

Whenever `wbs`, `wnt`, `wexp`, or `werr` processing occurs, the acquisition condition that initiated the processing is available from the parameter `acqstatus`. This acquisition condition is represented by two numbers: a "done" code and an "error" code. The done code is set in `acqstatus[1]` and the error code is set in `acqstatus[2]`. Macros can take different action depending on the acquisition condition. As an example, a `werr` macro could specify special processing if the maximum number of transients is accumulated. The appropriate test in the macro would be:

```
if (acqstatus[2] = 200) then
     "do special processing, e.g.dp='y' au"
endif
```

The acquisition codes and their meanings are listed in the description of the `acqstatus` parameter in the *VNMR Command and Parameter Reference*.

VNMR Error Messages

The `errlog` command displays a list of the most recent VNMR error messages in the text window. The global parameter `errloglen` controls the number of lines displayed. If `errloglen` is not defined, `errlog` displays 10 lines by default.

Noise Level Analysis

The command `noise<(excess_noise<,last_noise<,block_number>>)>` measures the noise level of a FID. Using `pw=0` so that no real signal is accumulated, you can acquire one (or more) transients. Usually about `np=4096` is sufficient. `noise` then performs a statistical analysis of the noise, informing you about noise level, dc level, etc. for each channel. This measurement can be repeated at various settings of `gain`, various settings of `fb`, etc., for a full system diagnosis.

If the `excess_noise` and `last_noise` arguments are included, they are used to calculate the noise figure: the first input argument is the excess noise, and the second is the last measured mean square noise. A third input argument can specify the block number (the default is 1).

The following arguments further define FID noise level measurement:

- `r1` returns the real dc offset.
- `r2` returns the imaginary dc offset.
- `r3` returns the real rms noise.
- `r4` returns the imaginary rms noise.
- `r5` returns the average rms noise.
- `r6` returns the percentage channel imbalance.

7.5 Applying Digital Filtering

The digital signal processing (DSP) capability of VNMR provides many benefits, such as constant noise level across the spectrum, improved integral accuracy, increased dynamic range, and flatter baselines. DSP usually involves the following three steps, all of which are automatically performed by the DSP software:

- The first step is to *oversample* the data. Oversampling means acquiring data with larger spectral width using a larger number of data points. For example, instead of collecting an 8-Kword data point set with a 5-kHz spectral width, a 160-Kword data set is acquired at 100 kHz. In DSP terms, this represents 20 times oversampling. An advantage of oversampling is that noise is reduced in situations where the noise in the time-domain FID is predominantly from round-off errors (“digitization errors”) in the analog-to-digital converter (ADC). This happens at low spectrometer gain settings, where the “real” noise being sampled by the ADC is small, perhaps less than 3 bits. Another advantage is that digital filters should cause less distortion of the FID, leading to many of the benefits of DSP mentioned in the introductory paragraph of this section.
- After the oversampled data is acquired, the next step is to apply a *digital filter* to the time-domain signal, or FID, to remove signals and noise at frequencies outside the final desired spectral width. Digital filters are defined by the filtering algorithm and the

number of coefficients for the filter. The more coefficients, the sharper the filter cutoff; however, the more complex the filter function and the greater the number of coefficients, the longer the calculation time required. In the example of oversampling above, the digital filter would be used to "cut-off" all frequencies outside the 5 kHz spectral width.

- The final step is to *downsample* the data. Downsampling (sometimes referred to as "decimation") means reducing the number of data points in the FID to the number actually required for spectral analysis at the chosen spectral width (the same number that you would have chosen if you had not used DSP). Again referring to the example above, the final FID would have 8-Kword data points and a final downsampled spectral width of 5 kHz.

Types of Digital Filtering

The main types of DSP provide digital filtering during the acquisition of data:

- Inline DSP uses software on the workstation to perform digital filtering and downsampling immediately after each oversampled FID is transferred from the console. Only the digitally filtered and downsampled data is written to disk. The advantages of the inline DSP include no increase in disk storage and user-defined filter functions. A potential disadvantage is some additional load on the workstation. Inline DSP software is compatible with all systems with Sun host computers.
- Real-time DSP uses a dedicated embedded processor chip installed on the input board of certain systems (such as the UNITY*INOVA*) to filter the data prior to time averaging. The advantages of real-time DSP include no increase in data storage and compatibility with ultra-rapid experiments (because there is no additional loading on the workstation). A disadvantage is that fewer parameters are available to control real-time digital filtering.

Another type of DSP, postacquisition DSP, integrates the digital filtering and downsampling process into the Fourier transform commands `ft` and `ft2d`. The digitally filtered and downsampled FID can then be saved to disk. The advantage is that the original FID is not altered in the original experiment, multiple applications of digital filtering are possible, no limitations exist on filter shape complexity and filter cutoff, and user-defined filter functions are possible. The main disadvantage is the large disk storage required. The usual disk storage requirements are directly multiplied by the oversampling factor, which ranges from 2 through 68. Postacquisition DSP software is compatible with all systems with Sun host computers.

In all types of DSP, the signal is initially filtered at the oversampled spectral width by an analog anti-aliasing filter.

Table 29 summarizes the commands and parameters associated with DSP.

Control of DSP

The value of parameter `dsp` specifies the type of DSP for data acquisition: `'i'` for inline DSP, `'r'` for real-time DSP, or `'n'` for none. As a global parameter, `dsp` affects DSP operation in all experiments and should be thought of as an hardware configuration parameter, because if DSP hardware is available (such as on the UNITY*INOVA*), that hardware is generally the method of choice.

Normally, DSP works quite invisibly to the user. Regardless of whether `dsp` is set to `'i'` or `'r'`, the oversampling factor (the parameter `oversamp`) is automatically set to the maximum allowed value whenever `sw` is entered. Thus, after the user enters `sw`, `at`, and/

Table 29. Digital Filtering Commands and Parameters

Commands	
`addpar('downsamp'|'oversamp')`	Add DSP parameters to the current experiment
`digfilt(exp_number<,option>)`	Write digitally filtered FIDs to another experiment
`movedssw`	Set parameters for digital filtering and downsampling
`moveossw`	Set parameters for digital filtering and oversampling
`pards`	Create digital filtering and downsampling parameters
`paros`	Create oversampling and digital filtering parameters
Parameters	
`at` {number, in seconds}	Acquisition time
`def_osfilt` {'a','b'}	Default value of `osfilt`
`downsamp` {number,'n'}	Downsampling factor applied after digital filtering
`dscoef` {number}	Digital filter coefficients for downsampling
`dsfb` {'n',number in Hz}	Digital filter bandwidth for downsampling
`dslsfrq` {number,in Hz}	Bandpass filter offset for downsampling
`dsp` {'i','r','n'}	Type of DSP for data acquisition
`filtfile` {file}	File of FIR digital filter coefficients
`fsq` {'n', 'y'}	Frequency-shifted quadrature detection
`np` {number}	Number of data points
`oscoef` {number}	Digital filter coefficients for oversampling
`osfilt` {'a', 'b', ''}	Oversampling filter for real-time DSP
`osfb` {'n', number, in Hz}	Digital filter bandwidth for oversampling
`oslsfrq` {number, in Hz}	Bandpass filter offset for oversampling
`oversamp` {'n',number}	Oversampling factor for acquisition
`sw` {number,in Hz}	Spectral width in directly detected dimension

or `np` in the normal manner, the software and hardware automatically oversamples at the maximum rate, and then digitally filters and downsamples the data according to the selected `sw` and `np` parameters.

If the user wishes to disable DSP for a particular experiment, the `oversamp` parameter can be set to `'n'` and oversampling and DSP are not be used. Or if desired, the `oversamp` parameter can be set by direct numeric entry to a value less than the maximum (e.g., `oversamp=4`). Be warned, however, that `oversamp` is reset to its maximum value the next time `sw` is entered in that experiment.

Inline DSP

Inline DSP applies digital filtering and downsampling to the acquired data prior to storage to disk on the host computer. Only the downsampled data set is stored using this method. DSP prior to data storage to disk has a time constraint: the digital filtering and downsampling must be completed within the time between transfer of successive data blocks (or increments of a 2D experiment) to the host computer disk. Additional processing done during acquisition, such as `wnt`, also adds to the time constraints. This processing can limit the speed of rapid arrayed experiments and depends on the type of Sun host computer and the parameters used.

Inline DSP is activated by setting the global parameter `dsp` to `'i'`. If `dsp` is not present or is set to `'n'`, DSP is disabled. If `dsp='i'`, setting the `oversamp` parameter to a value greater than 1 in a particular experiment causes the next experiment run to be oversampled, digitally filtered, and downsampled back to the selected `sw` prior to saving it to disk.

On the UNITY*INOVA*, inline DSP is completely compatible with interleaving and with stopping and restarting on acquisition with `sa` and `ra`. On systems other than UNITY*INOVA*, inline DSP is not possible if interleaving is active (`il='y'`). Also, the command `sa` can be used to stop acquisition, but `ra` cannot be used to resume it.

To Apply Inline DSP

1. Enter **`dsp='i'`**.

   This turns on inline digital filtering and calls the macro `paros` to create the oversampling parameters `oversamp`, `oscoef`, `oslsfrq`, `osfb`, and `filtfile`. While inline DSP is active, the filter bandwidth parameter `fb` is set to "Not Active."

2. Set parameters **`sw`** and **`at`** to the values desired for the final spectrum.

3. As required, adjust the values of the oversampling parameters **`oversamp`**, **`oscoef`**, **`oslsfrq`**, **`osfb`**, and **`filtfile`**:

   - `oversamp` specifies the oversampling factor (68 or less) for the acquisition. As a result, `np*oversamp` data points are acquired at a rate of `sw*oversamp`. Once the data has been transferred to the host computer, it is digitally filtered and downsampled to give `np` points and a spectral width of `sw`. `sw*oversamp` and `np*oversamp` are limited by the values given in Table 30. :

     Table 30. Maximum Values for `sw*oversamp` and `np*oversamp`

System	*Maximum* `sw*oversamp`	*Maximum* `np*oversamp`
UNITY*INOVA*	500 kHz	2M
MERCURY-VX, *MERCURY*	100 kHz	256 K
UNITY*plus*, UNITY, VXR-S	100 kHz	512K
GEMINI 2000 Broadband	100 kHz	128K
GEMINI 2000 $^{1}H/^{13}C$	23 kHz	64K

     The maximum `np*oversamp` is given for double precision data (`dp='y'`). For `dp='n'`, multiply the value by 2. The value of `oversamp` might need to be decreased further for rapid arrayed experiments, because of host computer memory and speed limitations. Setting `oversamp` to `'n'` causes normal acquisition to be done without digital filtering

   - `oscoef` specifies the number of coefficients used in the digital filter. The default is `7.5*oversamp+1`. A larger number of coefficients gives a filter with sharper cutoffs; a smaller number of coefficients gives a filter with more gradual cutoffs. The value of `oscoef` does not need to be changed when `oversamp` is changed because `oscoef` is automatically adjusted by VNMR to give filter cutoffs that are the same regardless of the value of `oversamp`.

   - `oslsfrq` is used to select a bandpass filter that is not centered about the transmitter frequency. `oslsfrq` is specified in Hz and works much like `lsfrq`. A positive value of `oslsfrq` selects a region upfield from the transmitter frequency, and a negative value selects a downfield region. The `oslsfrq` parameter can be used to perform frequency-shifted quadrature detection (see "Removing Quadrature Artifacts Using DSP" on page 218).

   - `osfb` specifies the digital filter bandwidth. If `osfb='n'`, the bandwidth defaults to `sw/2`. A value less than `sw/2` rejects frequencies at the edges of the

spectrum; a value more than `sw/2` aliases noise and signals at frequencies outside of `sw/2`

- `filtfile` specifies the name of a file of finite impulse response (FIR) digital filter coefficients. The file must be in the user's `vnmrsys/filtlib` directory. The filter coefficient file is a text file with one real filter coefficient per line. Complex filters are not currently supported. To use the default filter coefficients calculated by VNMR, `filtfile` should be set to the empty string (`''`, i.e., two single quotes with no space between them).

4. If `oversamp` is set to a value greater than 1, the next experiment is oversampled, digitally filtered, and downsampled to the `sw` selected prior to saving it to disk.

After acquiring a data set without digital filtering, the `moveossw` macro can be used to set `oslsfrq` and `sw` to appropriate values for oversampling and digitally filtering for the region of the spectrum selected between the cursors in the `ds` display. You must manually set `oversamp` to an appropriate value.

Real-Time DSP

Real-time DSP, available on certain systems (such as the UNITY*INOVA*), applies digital filtering during data acquisition, prior to storing the data in the memory of the acquisition computer. Data sampling is performed at a maximum rate of 400 kHz, with a maximum oversampling factor of 68. Thus, a typical 7-kHz spectrum is oversampled at a factor of 57; a 25-kHz spectrum is oversampled at a factor of 16. Above `sw=200000`, oversampling (and hence real-time DSP) is not possible and is automatically deactivated.

Oversampling lessens the effect of digitization noise on the spectrum, more so the more oversampling is done. At low gain, this can produce a marked improvement in the obtainable signal-to-noise (S/N) ratio. Equivalently, the use of oversampling and digital filtering will produce the same S/N at lower receiver gain values.

To Apply Real-Time DSP

When real-time DSP is first installed on a system, each user should enter `dsp?` to check that real-time DSP (`dsp='r'`) is set on the system. From that point on, the software automatically calculates oversampling factors and performs experiments using real-time DSP in a manner totally transparent to the user.

To turn DSP off in a single experiment, set `oversamp='n'`; to turn DSP back on in that experiment, set `oversamp='y'`.

To turn off DSP “permanently,” for all future experiments (until you decide to turn it back on again), set `dsp='n'`.

Types of Real-Time Digital Filters

Two different digital filters are supplied with real-time DSP. The first type, the Analog*Plus*™ filter, was designed to have similar characteristics to traditional analog filters, while using digital technology to improve on the analog filter in every way. The Analog*Plus* digital filter is flatter in the passband (the spectral region of interest) than an analog filter, and has sharper cutoff in the stopband (the region outside the spectrum to be filtered out). This gives better quantitation across more of the spectrum and reduced “noise fold-in” compared with analog filters, in addition to the improvement in S/N from the removal of digitization noise.

When comparing Analog*Plus* digital filters with analog filters (see Figure 65), note that when using a “real” analog filter, VNMR increases the filter bandwidth `fb` by 10%, compared with half the spectrum width, in order to provide better filter flatness across the spectral region of interest. This increase, however, causes significant noise to fold in to the spectrum. With the Analog*Plus* digital filter, however, the filter bandwidth (the 3-dB point) is set to exactly `sw/2` to ensure the best possible S/N across the spectrum.

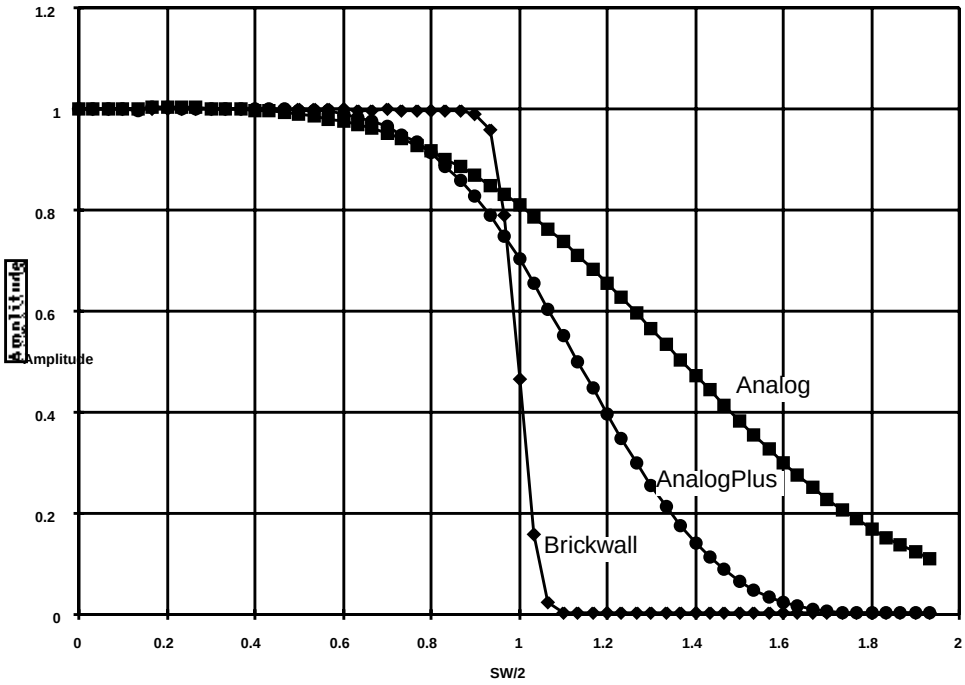


Figure 65. Digital Filters Compared to Analog Filters

The second type of digital filter provided, the Brickwall filter, has much sharper cutoff characteristics (as implied by its name) than the Analog*Plus* filter and is flatter even closer to the edges of the spectrum. This enhanced filtering may come at the expense of baseline performance, however. Users working with “simple” spectra, such as of organic compounds, should not notice this at all, but for work with high-dynamic range spectra or spectra of proteins, the baselines obtainable with the Brickwall filter may not be as good as the baselines obtained with the Analog*Plus* digital filter.

The global parameter `def_osfilt` specifies whether the digital filter you normally prefer is `'a'` (Analog*Plus*) or `'b'` (Brickwall). Once you set `def_osfilt`, you need not change it again. You can set a local parameter in each experiment, `osfilt`, to `'a'` or `'b'` to run a specific type of digital filter in that experiment, without changing your default choice.

The amount of oversampling performed by the system is contained in the parameter `oversamp`, which is normally calculated by the software to be the maximum possible for any given spectral width. You can change `oversamp` (to smaller values only) if you want to, but since the maximum benefit of DSP is only obtained with the maximum possible oversampling, there is little reason to do so.

For Brickwall filters, which use more coefficients than Analog*Plus* filters, some difference appears in the steepness of the filter as a function of the `oversamp` parameter. At `oversamp` set from 2 through 7, the cutoff is the steepest; as `oversamp` increases, the

filter becomes slightly less steep and approaches Analog*plus* filters at `oversamp=50`. Thus, if you want the flattest (in the passband) and sharpest (in the stopband) possible filter, and if you are not operating at low gain where oversampling is important to S/N, you may wish to use minimum oversampling (`oversamp` set from 2 through 7). Brickwall filters at oversampling factors of 20 to 40 make a nice compromise filter with better amplitude flatness than Analog*plus* and better baselines than Brickwall set at lower oversampling factors.

Real-Time DSP Details

Real-time DSP is not compatible with pulse sequences that use explicit acquisition to acquire less than the full number of data points (`np`) in a single `acquire` statement (e.g., solids sequences such as `br24` and `flipflop`). This incompatibility is taken care of automatically by the software, which turns off DSP and sets `oversamp='n'` if you attempt to acquire data using an incompatible pulse sequence. If you want to obtain the benefits of DSP in such experiments, use inline or postacquisition DSP.

Preserving the full potential dynamic range benefit of DSP for `dp='y'`, real-time DSP contains an inherent "gain" of 16 or the equivalent of 20 bits of data. A consequence of this gain is that if you look at the output of a single transient, the largest possible signal is no longer ±32768 (2^{16}) but instead ±524288 (2^{20}). In other words, the system behaves as if it has a 20-bit digitizer instead of a 16-bit digitizer.

For `dp='n'`, the "gain" of 16 mentioned above is disabled and, therefore, the main data value is 32767.

Another consequence of the gain with `dp='y'` is that if the ADC is filled on a single transient and the signals add coherently on successive transients (as they do in most experiments but not in, say, an indirect detection experiment), after a minimum of 4096 transients ($2^{32}/2^{20}$), the accumulating signal can overflow the available memory (the largest signal becomes greater than 2^{32} and cannot be stored in memory). The hardware does not prevent this overflow, and it is possible to obtain data that is useless in such a case. If you need to run more than 4096 transients, use inline or postacquisition DSP.

One subtle point involves ADC overflow on a single transient. When DSP and hence oversampling are activated, two changes occur that affect the maximum signal seen by the ADC. First, the initial sampling occurs earlier in time. The system may have acquired 10 points of an oversampled FID before it would have acquired a single point in a "normal" FID. Thus, any transient signals (e.g., probe background, pulse breakthrough) that occur at the front of the FID are more likely to cause ADC overflow in an oversampled FID. Second, the analog filter bandwidth is now set to a larger value—it may have gone from 2.5 kHz up to 50 kHz. Any large "out-of-band" signal that was being filtered out by the analog filter appears at the ADC to be digitized (and then to be subsequently filtered out by the digital filter). Thus again, ADC overflow may occur under conditions (i.e., identical pulse width and gain) where it did not occur when DSP was not used.

Even more subtly, because of the digital filtering that occurs, the output of the digital filter may actually have a value less than the maximum possible value, even though the input to the digital filter did indeed exceed the ADC limit. Thus, you should not be surprised if you occasionally need a very slightly lower gain to avoid ADC overflow when using DSP, and you should also not be surprised if you examine the (output) signal and do not see any evidence of ADC overflow, despite having been told by the software that ADC overflow did occur.

As explained earlier however, one of the real advantage of DSP with significant oversampling is the ability to work at lower gain settings while maintaining full signal-to-noise. This "headroom" afforded by DSP makes it is far less important to carefully adjust

the gain setting and fill the ADC. Thus, gain settings 6 to 10, or even 20 dB below ADC overflow, are likely to give perfectly acceptable results.

Data Format Issues

The output of inline and real-time DSP is a “normal” FID, without the distortion associated with the large frequency-dependent phaseshift associated with some digital filters, and with characteristics (such as `np`) that are identical to an FID obtained without DSP. As such, the output can be processed by any software (VNMR or third party) that can process standard VNMR FIDs. Real-time DSP FIDs are always in fixed point format (16- or 32-bit, depending on the value of the parameter `dp`).

The output of inline DSP is also a “normal” FID that can be processed in standard ways. If `dp='n'`, the FID is in a 16-bit fixed point format; however, if `dp='y'`, the FID is in 32-bit floating point format, not 32-bit fixed point.

VNMR processes such FIDs transparently, but some third-party software may not be compatible with this mode

Obtaining Good Baselines with Inline and Real-time DSP

The algorithms used by inline and real-time DSP processing now contain Varian’s time-corrected zero-phase digital filters. These filters allow very flat baselines to be obtained with no frequency dependent phase shift across the spectra. Getting these flat baselines does require some changes in setup and acquisition parameters from those used for analog filters.

Many users working with spectra of proteins are accustomed to using the `hoult` and `calfa` macros to adjust the acquisition conditions such that spectra are obtained with a frequency-dependent phase shift (`lp`) of zero and with minimal distortions of the second and subsequent data points with analog filters. These conditions are typically satisfied with negative values of `alfa`.

The same acquisition conditions do not result in the flattest possible baselines when using real-time DSP. The following procedure is recommended to set `alfa` and `rof2`:

1. Start by using “normal” positive values of `alfa` and `rof2`, (e. g., `alfa=6 rof2=2;` in fact, the software automatically sets these values the first time you activate DSP).
2. Obtain a spectrum and phase it properly.
3. Enter **`crof2`** to recalculate `rof2` so that `lp` will be zero.
4. Reacquire the spectrum to verify that `lp` is now zero.

After the last step, the baseline should be reasonably good. To improve it even further, you can make fine adjustments to `alfa` and `rof2`, keeping the sum of the two constant (e. g., enter `alfa=alfa-0.5 rof2=rof2+0.5 ga`). Once good values are obtained, you should find them relatively invariant with `sw` (as long as maximum oversampling is used).

The `calfa` macro has also been modified for used with DSP. `calfa` now sets `alfa` to the default value of about 6 µs and then adjusts `rof2` to set the appropriate timing for `lp=0`. If a value of `alfa` other than the default value is found to be preferable using the above methods, use `crof2` to adjust acquisition timing for the `lp=0` condition without changing the preferred value of `alfa`.

Postacquisition DSP

The software allows postacquisition digital filtering and downsampling to selectively detect a region of a spectrum. The digital filtered and downsampled FID can then be saved to disk. The digital filtering and downsampling processes are integrated into the `ft` and `ft2d` commands and occur when these commands are executed as specified by the parameters below. The digital filtering and downsampling are done just prior to the Fourier transform, so all apodization, linear prediction, solvent suppression, etc. are done prior to digital filtering.

Postacquisition digital filtering uses the same algorithm as inline DSP, with a transition bandwidth correction enhancement to minimize baseline distortion.

Application of postacquisition DSP takes the following steps:

1. Acquire a data set with `sw` = N*(final desired `sw`) and `np` = N*[(final desired `np`) + `dscoef/2`)], with N the oversampling factor.

   In most situations, you can use `np` = N*(final desired `np`) because the final `np` is usually much larger than `dscoef/2`.

2. After a data set has been acquired, enter the macro `pards` to create additional parameters `downsamp`, `dscoef`, `dslsfrq`, `dsfb`, and `filtfile` used by downsampling.

3. Setting up of the parameters can be made easier if an initial Fourier transform spectrum exists already. In this case, the macro `movedssw` can be used to set the parameters by using cursors in the `ds` spectral display. Position the vertical cursors around the region of interest and enter `movedssw`. Otherwise, set the parameters as follows:

   - `downsamp` specifies the downsampling factor applied after digital filtering. For example, starting with a spectral width of 100 kHz and `downsamp` set to 20, downsampling reduces the final spectral width to 5 kHz. The spectral width `sw` of the data set after digital filtering and downsampling is (acquired `sw`)/ `downsamp`. Setting `downsamp` to 1 allows digital filtering with a filter bandwidth specified by `dsfb` without downsampling. Setting `downsamp` to `'n'` allows normal data processing in VNMR without digital filtering.
   - `dscoef` specifies the number of coefficients used for filter computation. The default of 61 is usually a good choice. A larger number of coefficients gives a filter with sharper cutoffs, and a smaller number of coefficients gives a filter with more gradual cutoffs. Larger values in the range of 199 to 399 coefficients may have to be used to prevent aliasing of large peaks just outside the downsampled window. `dscoef` does not need to be changed as `downsamp` is changed, because `dscoef` is automatically adjusted by VNMR to give filter cutoffs that are the same regardless of the value of `downsamp`. This is done by actually using `dscoef*downsamp/2` coefficients in the digital filter. VNMR always rounds `dscoef*downsamp/2` to an odd number.
   - `dslsfrq` is used to select a bandpass filter that is not centered about the transmitter frequency (`tof`). `dslsfrq` is specified in Hz and works much like `lsfrq`. A positive value of `dslsfrq` selects a region upfield from the transmitter frequency and a negative value selects a downfield region. Bandpass filters are used to select regions away from the transmitter frequency.
   - `dsfb` specifies the digital filter bandwidth, which is set to half of the downsampled spectral width by default. If `dsfb='n'`, the default value for the filter bandwidth is used. A smaller value rejects frequencies at the edges of

the spectrum, and a larger value aliases noise and signals at frequencies outside of ± sw/2.

- `filtfile` specifies the name of a file of finite impulse response (FIR) digital filter coefficients. The file must be in the user's `vnmrsys/filtlib` directory. The filter coefficient file is a text file with one real filter coefficient per line. Complex filters are not currently supported. To use the default filter coefficients calculated by VNMR, `filtfile` should be set to the empty string (`''`, i.e., two single quotes with no space between them).

4. Once the parameters have been set, the filtered and downsampled dataset can be saved by using the macro `digfilt(exp_number<,option>)` to write the digitally filtered FIDs to another experiment. The data can then be saved by joining the other experiment and using the `svf` command to write the digitally filtered FID to disk. The possible options available with the `digfilt` macro are `'nodc'`, `'zero'`, and `'t2dc'`. Use these options if you used the same option when processing the data with `ft`, `wft`, `ft2d`, or `wft2d`. If `ct=1`, it may also be useful to use `dcrmv='y'` during data processing. If `proc='lp'`, linear prediction will be done prior to digital filtering. Apodization will also be done prior to digital filtering.
5. Carry out the digital filtering and Fourier transformation by entering `wft`, or in the case of 2D datasets, by entering `wft2d`. The digital filtering and downsampling step takes place after all other processing on the FID (dc, solvent suppression, linear prediction, apodization, etc.). If desired, the filtered downsampled data can be written to another experiment and then saved using the `svf` command.

Removing Quadrature Artifacts Using DSP

Normally, NMR spectra are acquired with the receiver in the center of the spectrum, and the center (zero) frequency glitch and quadrature artifacts fall within the desired spectral width. The use of the `oslsfrq` parameter with inline DSP allows these artifacts to be removed by the digital filter before downsampling so that they are not present in the downsampled FID that is stored on the disk. This technique is called frequency-shifted, or “digital,” quadrature detection.

Frequency-shifted quadrature detection is accomplished by moving `tof` to just outside the desired spectral width and then using `oslsfrq` to offset the digital filter center frequency by the same amount, thus keeping the region of interest after digital filtering. Frequency-shifted quadrature detection is done in the inline DSP algorithm.

- If real-time DSP is used (`dsp='r'`), `oversamp` is set to a multiple of 4, and downsampling of a factor of `oversamp/4` is then done in real-time DSP. The remaining factor of 4 is then done in inline DSP, during which frequency-shifting by `oslsfrq` is also done. This feature is available only on UNITY*INOVA* systems.
- If pure inline DSP is used (`dsp='i'`), filtering and frequency-shifting is done in a single stage.

To Apply Frequency-Shifted Quadrature Detection

UNITY*INOVA Systems*

1. Turn DSP on by setting `dsp` to `'r'` or `'i'`.
2. Set **`fsq='y'`**.

Doing these steps sets `oslsfrq` to `1.25*sw` and offsets the transmitter frequency to `tof+oslsfrq` just before acquisition. If a different value of `oslsfrq` is desired, it can be entered after `fsq` is set to `'y'`.

MERCURY-VX and MERCURY Systems

1. Because only inline DSP is available, set `dsp='i'`.
2. Set **`fsq='y'`**.

Doing these steps sets `oslsfrq` to `1.25*sw` and offsets the local oscillator from the transmitter by `oslsfrq` when the transmitter frequency is set. This occurs at the beginning of the pulse sequence, or any time the transmitter frequency is set. If a different value of `oslsfrq` is desired, it can be entered after `fsq` is set to `'y'`.

On systems other than UNITY*INOVA*, *MERCURY-VX*, and *MERCURY*, inline DSP with `oslsfrq` can be used.

1. Set **`dsp='i'`**.
2. Set `oslsfrq` to `1.25*sw`, and move `tof` by the same amount.

   To move `tof`, you can add two statements to the relevant pulse sequences to shift the transmitter to the center of the spectrum (`tof`) at the beginning of the pulse sequence, and then shift the transmitter to the position offset by `oslsfrq` for data acquisition. For example:

   ```
   status(A);
   obsoffset(tof);
   delay(d1);
   ...
   obspulse(pw,oph)          /* last pulse in sequence */
   obsoffset(tof+oslsfrq);
   ```

3. Enter **`fsq='y'`** to set `oslsfrq`.

Setting Frequencies

For pulse sequences that explicitly use a frequency other than `tof` during acquisition, the appropriate frequencies need to be set in a similar fashion.

Frequency setting is automatically done on *MERCURY-VX* and *MERCURY*. To set frequencies on other systems, add the pulse sequence statements, and set `oslsfrq` to `1.25*sw`. On UNITY*INOVA*, you must also set `fsq='n'`. Keep in mind that in most pulse sequences, to get best use of pulse power, the transmitter frequency during pulses should be kept in the center of the spectrum, especially for 180-degree pulses.

Chapter 8. Data Processing

Sections in this chapter:

- 8.1 “Weighting Function” this page
- 8.2 “Interactive Weighting” page 223
- 8.3 “Fourier Transformation” page 223
- 8.4 “Phasing” page 224
- 8.5 “Advanced Data Processing” page 226

After data are acquired, the next step in the process is applying a “weighting function” to the FID, which is an optional part of the process, and Fourier transformation, which is not. Both processes are accomplished together with the command `wft` (weight and Fourier transform) command; the command `ft` performs only the Fourier transform and skips the weighting step.

8.1 Weighting Function

Table 31 lists weighting and Fourier transform parameters and commands. The weighting function used is governed by the following parameters:

- `lb` results in exponential weighting. A positive value gives the desired line broadening in Hz, which is then used to calculate a decaying exponential function. A negative value gives a resolution enhancement function.
- `gf` is a Gaussian time constant, in seconds, and defines a Gaussian function of the form `exp(-(t/gf)2)`.
- `gfs` shifts the center of the Gaussian function `exp(-((t-gfs)/gf)2)`.
- `sb` is a sinebell constant, in seconds. A positive value applies a sinebell of the form `sin(t*p/(2*sb))`. A negative value applies a squared sinebell function of the form `sin2(t*p/(2*sb))`.
- `sbs` is a sinebell shift constant, in seconds. It allows shifting the origin of the sinebell function according to the formula `sin((t-sbs)*p/(2*sb))`. Again, the square of this function is applied if `sb` is negative.
- `awc` is an additive weighting constant that adds the constant `awc` to each value of the weighting function. It is applied *after* the sinebell and exponential function but *before* the Gaussian function.

All these weighting functions can be applied simultaneously to the data. That is, one does not first apply a decreasing exponential function, then apply a convolution difference function, etc. Instead, all weighting functions to be used are set, and then are applied simultaneously as part of the `wft` command. To remove a particular weighting function from use, its value should be set to `'n'` (for not used). Its value is then displayed on the screen by `dg` as “not used.”

Table 31. Weighting and Fourier Transform Commands, Macros, and Parameters

Commands	
`ft*`	Fourier transform 1D data
`resolv<(a,b)>`	Set resolution enhancement parameters
`wft*`	Weight and transform 1D data
`wti<(element_number)>`	Interactive weighting
`* ft<(options,><'nf'><,start><,finish><,step>)>, ft('inverse',exp_num,expansion) wft<(options,><'nf'><,start><,finish><,step>)>, wft('inverse',exp_num,expansion)`	
Macros	
`gaussian`	Set up unshifted Gaussian window function
`pi3ssbsq`	Set up pi/3 shifted sinebell-squared window function
`pi4ssbsq`	Set up pi/4 shifted sinebell-squared window function
`sqcosine`	Set up unshifted cosine-squared window function
`sqsinebell`	Set up unshifted sinebell-squared window function
Parameters	
`awc` {'n', number}	Additive weighting const. in directly detected dimension
`dcrmv` {string}	Remove dc offsets from FIDs in special cases
`fn` {power of 2 number}	Fourier number in directly detected dimension
`gf` {'n', number in sec}	Gaussian function in directly detected dimension
`gfs` {'n', number}	Gaussian shift constant in directly detected dimension
`lb` {'n', number}	Line broadening in directly detected dimension
`math` {'i', 'f'}	Fourier transform mathematics
`sb` {'n', number}	Sinebell constant in directly detected dimension
`sbs` {'n', number}	Sinebell shift constant in directly detected dimension
`wtfile` {'', file}	User-defined weighting in directly detected dimension

Although the system allows the combination of sinebell, exponential and Gaussian weighting, a combination of those can be difficult to understand and should only be used after experimenting with the individual parameters. The use of either Gaussian apodization (with `gfs='n'`), which leads to Gaussian line shapes, or line broadening (with `lb` greater than 0), which leads to Lorentzian lineshapes, is especially critical for deconvolution.

Other line shapes cannot be handled by the deconvolution program, but may be appropriate for 1D resolution enhancement or in absolute-value 2D experiments. In any case, weighting affects the integrals of different lines in different ways, and should be used with great care if quantitative results are requested.

The command `resolv<(a,b)>` sets defaults of `a` equal to 0.1 and `b` equal to 0.3 into the formulas `lb=-0.318/(a*sw)`, and `gf=b*sw`, thereby calculating “reasonable” values for the resolution enhancement parameters `lb` and `gf`. The arguments `a` and `b` can also be selected by the user.

Several macros exist that set weighting parameters to give certain window functions. These include `gaussian`, `pi3ssbsq`, `pi4ssbsq`, `sqcosin`, and `sqsinebell`.

The parameter `wtfile` is available for handling user-written weighting functions; see the manual *VNMR User Programming* for details

8.2 Interactive Weighting

The `wti` command allows interactive setting of weighting parameters (`lb, gf, gfs, sb, sbs`, and `awc`). If `wti` is called with an `index` number as an argument (e.g., `wti(3)`), the desired FID number in a multi-FID experiment is selected; otherwise, the current index is used.

To start `wti` from the menu system, select Adj Weighting in the 1D Data Processing Menu, in the 2D Data Processing Menu, or in the 2D Interferogram Processing Menu

During the `wti` display, a single menu with the following buttons is active (this menu is not user programmable):

Each button in this menu functions as follows:

next fid	Increments the FID/interferogram index.
lb	Selects line broadening or exponential weighting. A negative value gives resolution enhancement.
sb	Selects the sinebell constant. A negative value gives squared sinebell.
sbs	Selects the sinebell shift constant (only if sinebell is active).
gf	Selects the Gaussian time constant.
gfs	Selects the Gaussian time constant shift (only if Gaussian time constant is active).
awc	Selects the additive weighting constant.
return	Returns to the last menu before `wti` was entered.

Currently active weighting parameters can be changed by moving the mouse cursor to the appropriate field in the weighting function box and pressing the left mouse button. New values for weighting parameters can also be typed in. Note that all other parameters, unless set to “not used”, are also used to calculate the weighting function.

To adjust FID intensity (parameter `vf`), use the center mouse button within the FID box. To adjust spectrum intensity (`vs`), use the center mouse button within the spectrum box.

The right mouse button turns off and on the display of the transformed spectrum, useful for modifying the weighting function on slow terminals or large spectra.

8.3 Fourier Transformation

The `ft` command Fourier transforms one or more FIDs without weighting applied to the FID. To perform the same Fourier transform with weighting, use the command `wft`. Both `ft` and `wft` perform a shift and phase rotation according to the parameters `lsfid` and `phfid`, if these are set. Any dc level in the FID is automatically calculated and removed, except when `wft('nodc')` is used. Alternatively, the parameter `dcrmv` uses hardware information to remove the dc offset values from the FID when `ct=1`.

For the Fourier transformation process, the parameter `fn` is the number of points to be Fourier transformed. Because of the type of algorithm used, this number must be a power of two; typical numbers are 16384, 32768, or 65536 (often written as 16K, 32K, and 64K, where K is equivalent to multiplying the number by 1024). The most common entry for `fn` is `'n'`. This value specifies that however many data points (`np`) were acquired, the first

power of two greater than or equal to `np` will be used as `fn`. If `fn` is greater than `np`, or if `fn` is `'n'` and `np` is not a power of two, the remaining points in the transform are filled in with values of zero (*zero-filling*). Thus there is no explicit zero-filling command; this process is an implicit one governed by `fn`.

8.4 Phasing

Phasing spectra may be considered part of either data processing or data display; we treat it here as part of data processing. Table 32 lists spectral phasing software tools.

Table 32. Phasing Spectra Commands and Parametersn

Commands	
`aph<(args)><:ok,rp,lp>`	Automatic phase of rp and lp
`aph0<(args)><:ok,rp,lp>`	Automatic phase of zero-order term
`aphx`	Perform optimized automatic phasing
`av`	Set absolute-value mode in directly detected dimension
`ds<(index)>, ds<(options)>`	Display a spectrum
`ph`	Set phased mode in directly detected dimension
`phase(phase_change)`	Change frequency-independent phase rp
`pwr`	Set power mode in directly detected dimension
Parameters	
`lp` {–3600 to +3600 in degrees}	First-order phase in directly detected dimension
`rp` {–360 to +360 in degrees}	Zero-order phase in directly detected dimension

Performing a complex Fourier transformation produces two sets of data, referred to as the *cosine* and *sine* transforms, or the *real* and *imaginary* channels, respectively. In almost all cases, the absorption spectrum (peaks “in-phase”) and the dispersion spectrum (peaks “out-of-phase”) do not coincide with the real and imaginary channels, but must instead be produced from a linear combination of the two channels.

Phase Parameters

The process of phasing a spectrum requires the determination of an angle θ that can be used to “mix” these two data sets to produce one data set, according to the formula:

$$\textit{absorption spectrum}_{\omega} = \textit{real channel}_{\omega} * \cos\theta + \textit{imaginary channel}_{\omega} * \sin\theta \qquad \text{[Eq. 3]}$$

The process is complicated by the fact that phase angle θ is a function of frequency:

$$\theta = \texttt{rp} + (\omega - \omega_0) * \texttt{lp} \qquad \text{[Eq. 4]}$$

where `lp` (left or first-order phase) and `rp` (right or zero-order phase) are constants that must be determined.

The following is clear about the terms in Equation 4:

- `rp` is *frequency independent*. Changes in `rp` affect all peaks in the spectrum equally.
- `lp` is *frequency dependent*. Changes in `lp` affect peaks with a differing amount as a function of frequency.

There are several ways in which `lp` and `rp` can be adjusted:

- Like any parameter, they can be recalled with a particular parameter set. Once entered, they can also be entered directly (e.g., `lp=–150`).

- Fully automatic phasing is also provided with the aph command, which optimizes both the frequency-dependent (lp) and the frequency-independent (rp) parameters, and is independent of the starting point. The aph0 command only adjusts rp. The aphx macro optimizes parameters and arguments for the aph command. aphx first performs an aph then calculates a theoretical value for lp. If lp set by the aph is different from the calculated value by 10 per cent, the calculated value is used and an aph0 is performed.

The command phase(phase_change) changes the phase of all peaks in the spectrum by adding phase_change to the current value of rp, then removing any excess in rp more than 360°.

Autophase Algorithm

The automatic phasing algorithms aph and aph0 have been enhanced in several ways:

- Weighting parameters no longer affect the algorithms.
- Spectra with very low signal-to-noise can be phased.
- In vivo spectra can be phased. These spectra are very difficult for most autophasing algorithms.
- Spectra with inverted lines can be phased. Such spectra includes DEPT experiments or selectively inverted lines obtained with shaped pulses. This type of phasing is difficult for traditional autophasing algorithms, which cannot distinguish when a line is inverted and when a line is normal.

An autophasing algorithm uses many rules that are used in a manual phasing procedure. First, it finds the peak areas. Then, it estimates the correct phase for each peak. An initial guess of the first order phasing parameter lp is made based on the estimated phases of two "normal" peaks. The peaks are categorized into three classes: normal, inverted, and bad. The peaks in the normal and inverted group will be used to find the optimal values for the phasing parameters lp and rp. A final check is made to determine whether autophasing was successful or unsuccessful.

Algorithms are complicated but fairly "intelligent." The key point of an algorithm is to use a set of fuzzy rules to estimate the correct phase for each peak. The use of these rules makes an algorithm less sensitive to the signal-to-noise ratio, weighting parameters, and the base line quality. Fuzzy logic also makes it possible to do the classifications on the peaks.

The command aphb autophases Bruker data. Refer to the *VNMR Command and Parameter Reference* for more information about this command.

Spectrum Display

The displayed spectrum is calculated in one of three *mutually exclusive* modes:

- The *phase-sensitive mode* is selected by the command ph. In this mode, the displayed spectrum is calculated using the phase parameters lp and rp.
- The *absolute-value mode* is selected by the command av. In this mode, the displayed spectrum is calculated according to the equation

  $$absorption\ spectrum(\omega) = (real\ channel^2(\omega) + imaginary\ channel^2(\omega))^{1/2}$$

- The *power mode* is selected by the command pwr. In this mode, the displayed spectrum is the square of the displayed spectrum calculated in the absolute value mode.

Once a spectrum is displayed using the interactive display command ds, the spectrum can be interactively phased by selecting the Phase button from the menu (see Chapter 9,

"Display, Plotting, and Printing," for details). Any integral and cursors displayed along with the spectrum are removed.

8.5 Advanced Data Processing

This section covers advanced data processing, including phase rotation, frequency shifting, linear prediction, and interleaving FIDs. Table 33 lists the tools discussed.

Table 33. Advanced Data Processing Commands and Parameters

Commands	
`addpar('lp')`	Create parameters for linear prediction in np dimension
`addpar('ss')`	Create parameters for time-domain solvent subtraction
`dglp`	Display group of linear prediction parameters
`ilfid`	Interleave FIDs during data processing
`parfidss`	Create parameters for time-domain solvent subtraction
`parlp`	Create parameters for linear prediction in np dimension
`tmove`	Left-shift FID to time-domain cursor
Parameters	
`lpalg` {'lpfft','lparfft'}	Linear prediction algorithm in `np` dimension
`lpext` {number}	Linear prediction data extension in `np` dimension
`lpfilt` {number}	Linear prediction coefficients to calculate in `np` dim.
`lpnupts` {number}	Linear prediction number of data points in `np` dim.
`lpopt` {'b','f'}	Linear prediction algorithm data extension in `np` dim.
`lpprint` {number}	Linear prediction print output in `np` dimension
`lptrace` {number}	Linear prediction output spectrum
`lsfid` {'n', number}	Number of complex points to left-shift `np` FID
`lsfrq` {number, in Hz}	Frequency shift of the fn spectrum in Hz
`phfid` {–360 to +360, in deg.}	Zero-order phasing constant for np FID
`proc` {'ft','rft','lp'}	Type of processing on `np` FID
`ssfilter` {'n', 10 to sw/2, in Hz}	Full bandwidth of digital filter to yield a filtered FID
`sslsfrq` {'n', number in Hz}	Center of solvent-suppressed region of spectrum
`ssntaps` {1 to np/4}	Number of coefficients in the digital filter
`ssorder` {'n', 1 to 20}	Order of polynomial to fit digitally filtered FID
`strtext` {1 to np/2}	Starting point for linear prediction data ext. in `np` dim.
`strtlp` {number}	Starting point for linear prediction calculation

FID Phase Rotation

The parameter `lsfid` is a constant used in left-shifting the FID. If `lsfid` is set to a value other than `'n'`, the FID is left-shifted by `lsfid` complex points before weighting or Fourier transformation is performed. The value for `lsfid` must lie between `0` and `np/2`.

The parameter `phfid` is a zero-order FID phasing constant. If `phfid` is set to a value other than `'n'`, the FID is phase rotated by `phfid` degrees before weighting or Fourier transformation is performed.

The `tmove` macro provides a method of setting the parameter `lsfid`—position the right time cursor at the place that should be the start of the FID, then enter `tmove` to adjust the parameter `lsfid`.

Frequency Shifting

The parameter `lsfrq` sets a frequency shift of spectral data, in Hz, with a negative value resulting in peaks being shifted upfield (to the right) and a positive value in peaks being shifted downfield (to the left). `lsfrq` operates in the time domain on complex FID data, and thus must be entered *before* any Fourier transformation is performed.

Data Processing Methods

All data processed in VNMR is processed using the method of Fourier transformation, but there are three variations that are governed by the `proc` parameter:

- Most NMR data—including all data acquired on *MERCURY-VX*, *MERCURY*, UNITY*INOVA*, UNITY*plus*, *GEMINI 2000*, UNITY, VXR, and Gemini spectrometers—is acquired using *simultaneously* sampled ("true") quadrature detection. This means that two orthogonal (real and imaginary, or *x* and *y*, as you prefer) data points are sampled at the same time and form a single complex data point in the FID. Such data are processed using a normal complex Fourier transformation, using `proc='ft'`.
- Some spectrometers, notably those from Bruker Instruments, acquire pseudo-quadrature data by sampling two orthogonal data points *sequentially*, rather than simultaneously. Such data must be processed using a real Fourier transformation, with `proc='rft'`. Use `convertbru` to convert Bruker data (see Chapter 10, "Storing, Retrieving, and Moving Data," for details).
- For simultaneously sampled data only, it is possible to include as part of the Fourier transform process a "linear prediction," described in the next section. `proc='lp'` is used to trigger this operation.

Linear Prediction

Raw time-domain data acquired during a pulsed NMR experiment can have two flaws:

- Early points in the FID may be distorted due to a host of hardware characteristics, such as preamplifier saturation, probe ringing, and filter non-linearities. Even on a perfect spectrometer, these distortions cannot always be avoided.
- The acquisition time of each FID may have been too short to allow for full decay of the signal, leading to distortion in the Fourier transformed spectrum.

Both types of distortions can be solved using *linear prediction*. This uses the "good" part of the FID to analyze for the frequencies that are present in the signal, and then uses that information to extend the FID either in a reverse direction (to "fix" the first few "bad" points) or in a forward direction (to eliminate truncation problems). Following this process, the "new, improved" FID is then Fourier transformed in the usual way.

In VNMR, linear prediction is incorporated directly into the Fourier transform routine, so that normally one does not see the "improved" FID, but merely the spectrum which results from Fourier transforming the linear predicted FID. This is accomplished by setting `proc='lp'` and then entering `ft` or `wft` as usual. If you do wish to see the linear predicted FID, it is possible to do so by entering `ft('noft')`, which performs all the steps of the Fourier transform routine except the actual Fourier transformation. You can now see the real points of the FID by setting `lp=0 rp=0`, or see the imaginary points by setting `lp=0 rp=90`.

Since linear prediction involves solving a series of equations for appropriate coefficients based on the actual FID, it involves quite a number of parameters and can be somewhat

tricky to optimize (if not optimized properly, or if the data are not amenable, the analysis may simply fail, just like any least-squares fit process may fail to converge).

The parameters required for linear prediction do not exist in standard parameter sets, but can be created with the macro `addpar('lp')` and displayed with `dglp` (the macro `parlp` functions the same as `addpar('lp')`). Refer to Table 33 for a list of linear prediction parameters. Each parameter is described in detail in the manual *VNMR Command and Parameter Reference*.

For more complex problems, linear prediction can even be run in a iterative fashion—first extending backward, then forward, and perhaps again backward.

Users desiring more information on the algorithm implemented in the software, and on linear prediction in general, are referred to H. Barkhuijsen, R. de Beer, W.M.M.J. Bovée, and D. van Ormondt, *J. Magn. Reson.*, **61**, 465-481 (1985).

Solvent Subtraction Filtering

Numerous solvent suppression pulse sequences exist that reduce the signal from a large solvent peak to a level where the desired resonances can be observed. Often, however, experimental solvent suppression does not entirely eliminate an unwanted solvent peak. Digital filtering of the data can further suppress or eliminate a solvent peak.

VNMR incorporates two algorithms for solvent subtraction by digital filtering:

- In the first, called lfs (low-frequency suppression), a low-pass digital filter is applied to the acquired FID. This filter severely attenuates all signals that lie outside the passband of the filter, leaving only the on-resonance solvent signal and other low-frequency signals that fall within the filter bandwidth. This filtered FID is then subtracted from the original FID to remove the solvent peak contribution. The Fourier transform of this FID gives the solvent-subtracted spectrum.
- In the second, called zfs (zero-frequency suppression), the acquired FID is also low-pass filtered, but then the filtered FID is fit with a polynomial (specified by the parameter `ssorder`), and the polynomial is subtracted from the original FID. This has the effect of removing from the FID only the signal that is exactly on-resonance. The Fourier transform of this FID produces the solvent-subtracted spectrum.

The solvent subtraction parameters `ssfilter`, `sslsfrq`, `ssntaps`, and `ssorder` control processing. If these parameters do not exist in the current experiment, they can be created by entering `addpar('ss')`.

The parameters `ssfilter` and `ssorder` select the processing option as follows:

- The zfs (zero-frequency suppression) option is selected if both `ssfilter` and `ssorder` are set to a value other than “Not Used.”
- The lfs (low-frequency suppression) option is selected if `ssfilter` is set to a value other than “Not Used” and `ssorder` is set to “Not Used.”
- The zfs and lfs options are both turned off if `ssfilter` is set to “Not Used.”

The characteristics of the low-pass digital filter used with the lfs and zfs options can be modified by changing the parameters `ssfilter`, `sslsfrq`, and `ssntaps`:

- The value of `ssfilter` specifies the full bandwidth of the low-pass filter applied to the original FID to yield a filtered FID. Its default value is 100 Hz.
- The value of `sslsfrq` specifies the location of the center of the solvent-suppressed region of the spectrum. Setting `sslsfrq` to a non-zero value shifts the solvent-suppressed region by `sslsfrq` Hz. Setting `sslsfrq` to `'n'` (the default value) solvent suppresses a region centered about the transmitter frequency.

- The value of `ssntaps` specifies the number of taps (coefficients) used for the digital filter. The default value is 121 but the value can range from `1` to `np/4`. The more taps in a filter, the flatter the passband response and the steeper the transition from passband to stopband, giving a more rectangular filter. For the lfs (low-frequency suppression) option, the default is suitable. For the zfs (zero-frequency suppression) option, a value between 3 and 21 usually works better.

Additionally, if the zfs option is selected, the parameter `ssorder` specifies the order of the polynomial used to fit the digitally filtered FID. The order can range from 1 to 20. The default value is "Not Active." If the lfs option is selected, `ssorder` is not used.

The quality of filtering with zfs diminishes rapidly as the solvent peak moves off the exact center of the digital filter. It may be necessary to adjust `lsfrq` or `sslsfrq` to move the solvent peak to within ± 0.2 Hz of the center of the filter to obtain optimal solvent suppression. The lfs option is less sensitive to small offsets, but typically removes or distorts peaks near to the solvent peak.

Interleave FIDs

The `ilfid` command converts a multiple FID element into a single FID by interleaving the FIDs. When invoked in an experiment of `nf` FIDs, each of `np` points, `ilfid` sorts the data into a single FID of `np*nf` points that can then be transformed. The interleaving takes the first complex point of each of the `nf` FIDs and places them in sequential order in the new FID. It then takes the second complex point from each of the `nf` FIDs and appends them sequentially to the new FID. This operation is repeated for all complex points. Although `ilfid` adjusts `np` and `nf`, it does not alter other parameters such as `sw`.

CAUTION: **Because ilfid alters the data irrevocably, it is strongly recommended that you save the FID before using ilfid.**

For further information on `ilfid`, including an example, refer to the *VNMR Command and Parameter Reference*.

Chapter 9. Display, Plotting, and Printing

Sections in this chapter:

- 9.1 “Interactive FID and Spectrum Display” this page
- 9.2 “Interactive FID Display” page 233
- 9.3 “Stacked and Whitewashed FID Display and Plotting” page 236
- 9.4 “Interactive Spectrum Display” page 237
- 9.5 “Spectral Display and Plotting” page 243
- 9.6 “Integration” page 250
- 9.7 “Plotting” page 254
- 9.8 “Plot Designer” page 262
- 9.9 “Printing” page 271
- 9.10 “User-Controllable Line Drawing” page 272

Display, plotting, and printing of data are highly individualized activities. Each user has their own ideas about proper formats, necessary expansions, etc. For this reason, this chapter more than any other should probably be read from beginning to end.

9.1 Interactive FID and Spectrum Display

The interactive display programs covered in this chapter are the `df` program for FID display and the `ds` program for spectrum display. In the displays of these programs, you can interact with the FID or spectrum in three different ways:

- Each mouse button can be labeled with the name and value of some display parameter; different parameters are present depending upon the nature of the display. These labels are highlighted in the lower right corner of the display screen. Clicking a mouse button produces a change in the corresponding parameter.
- Parameter values can be entered “by hand.” For example, typing `vs=500` will change the vertical scale of the displayed spectrum to 500 mm. It is not necessary to “exit” the “display mode” and enter a “parameter entry mode” to do this.
- Each function key can cause a different change in the display. Labels for the function keys are always displayed at the top of the display screen. The action associated with each function key may be invoked by pressing the appropriate function key on the keyboard or by moving the mouse arrow to the appropriate label and clicking a mouse button. Using function keys, it is possible to take actions, such as display one or two cursors, to rapidly expand the region between two cursors, to adjust the start and width of the displayed FID or spectrum, and to return to the menu system.

Function keys that cause a change in display mode (for example, add a cursor to the display) may also cause a reassignment of the mouse buttons. In each case, the mouse button will

be changed, with the name of the parameter it controls. Until you have used the system for some time, it is a good idea to look at the mouse labels before you click a mouse button to make sure you are changing the parameter you intend to change.

Display Parameters

FID and spectral display is governed by a number of parameters. The FID region displayed is determined by the "plot" parameters `wf` (width of FID) and `sf` (start of FID). Similarly, the spectral region displayed is determined by the parameters `wp` (width of plot) and `sp` (start of plot). These parameters are entered in seconds and Hz respectively (e.g., `wp=1000`).

Display of these parameters is controlled by the parameter `axisf` (for FID display) or `axis` (for spectrum display); these are also used to regulate the labeling of plot scales, peak frequencies, etc. `axisf` is typically in seconds; `axis` is typically in either `p` (ppm), `h` (Hz), or `k` (kHz). For FID display, the parameter `vf` affects the vertical scale of the display.

For spectrum display, the parameter `vs` affects the vertical scale. Scale intensities depend on the display mode:

- In the normalized (`nm`) display mode, the largest peak in the spectrum is automatically found, then the display is normalized to make the peak `vs` mm high on the plot.
- In the absolute-intensity (`ai`) mode, the appearance on the display screen is used as a guide to adjust `vf` or `vs` to produce the desired vertical scale. This mode enables comparing intensity from one experiment to another, a necessity for *all* arrayed experiments.

The position of the display on the screen and the plotter is governed by the "chart" parameters, `wc` (width of chart) and `sc` (start of chart). Both are entered in units of millimeters. For FID display, the parameter `vpf` positions the FID display vertically; for spectrum display, the parameter `vp` positions the spectrum vertically and `io` (integral offset) positions the integral with respect to the spectrum (in units of millimeters).

Plotting

The general rule of plotting is that "what you see is what you get;" the data that is displayed on the screen, or would be displayed on the screen if you type `df` or `ds`, is what will be plotted on the page. This rule applies not only to the FID or spectrum but to the positioning of each as well. In other words, if the parameters are set to plot the FID or spectrum on the left half of the plotted page, then a display of the spectrum will similarly display the FID or spectrum on the left half of the screen.

Vertically as well, full scale on the screen represents full scale on the plotter. This relationship is used to adjust the vertical scale in `ai` mode, since in that case `vf` or `vs` is not the height of the largest peak. In `nm` mode, this fact is also used in cases in which the largest peak is desired to be off-scale.

An exception to the general rule of plotting is provided by the `wysiwyg` parameter. If you would prefer to scale the image to the full window, which should be easier to view, set `wysiwyg` to `'n'`. This setting scales the window but does not change the ratio of the image. To return to the normal "what you see is what you get" display, change `wysiwyg` to `'y'`.

9.2 Interactive FID Display

The `df<(index)>` command, or the equivalent command `dfid<(index)>`, enables interactive manipulation of a single FID. For arrayed 1D experiments or for 2D experiments, a particular FID can be viewed by supplying the index number as an argument. From the menu system, this program is opened by selecting the button Display FID in the 1D Data Processing Menu.

The FID is left shifted by the number of complex data points specified by the parameter `lsfid`. The FID is also phase rotated (zero-order only) by the number of degrees specified by the parameter `phfid`.

Table 34 lists commands and parameters associated with the interactive FID display.

Table 34. Interactive FID Display Commands and Parameters

Commands	
`df<(index)>, df<(options)>`	Display a single FID
`dscale*`	Display scale below spectrum or FID
`* dscale<(<axis><,vertical_start><,display_start><,color>)>`	
Parameters	
`axisf` {'s','m','u','n'}	Axis label for FID displays and plots
`crf` {number, in sec}	Current time-domain cursor position
`deltaf` {number, in sec}	Difference of two time-domain cursors
`lsfid` {'n', number}	Number of complex points to left-shift np FID
`phasing` {10 to 100, in %)	Control update region during interactive phasing
`phfid` {'n',–360.0 to 360.0, in deg.}	Zero-order phasing constant for np FID
`vf` {1e–6 to 1e9}	Vertical scale of FID
`vpf` {number, in mm}	Current vertical position of FID
`vpfi` {number, in mm}	Current vertical position of imaginary FID

FID Display Menu

Figure 66 shows a typical display with a FID and a single vertical cursor.

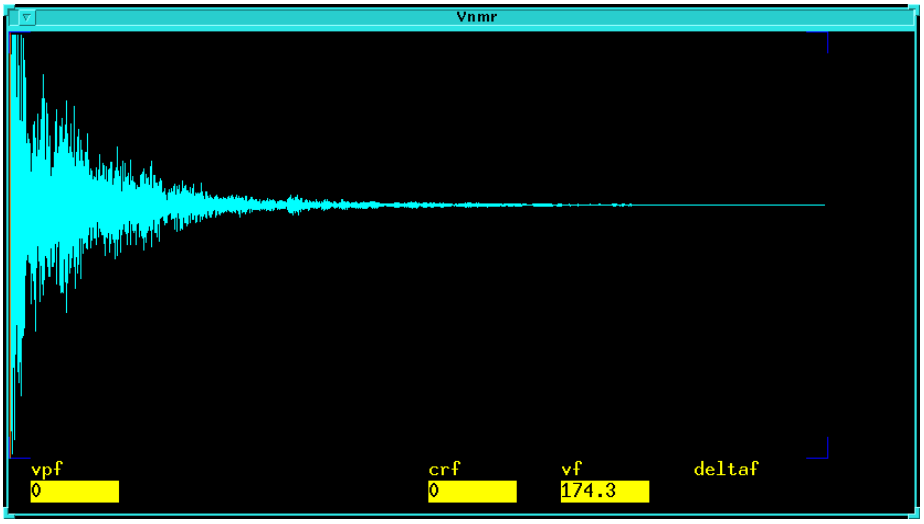


Figure 66. Interactive FID Display (`df` Program)

At the top of the display is the FID Display Menu with the following buttons (note that the labels change on some of the buttons according to the mode the program is in):

These buttons function as follows:

The first button is Box or Cursor, depending on if you are in the box or cursor mode:

Box	Change to the box mode with two cursors.
Cursor	Change to the cursor mode with one cursor.

The second button is Imaginary, Zero Imag, or No Imag, depending on which mode you are in:

Imaginary	Display the imaginary FID.
Zero Imag	Display the imaginary FID as all zero.
No Imag	Remove the imaginary FID display.

The third button is Expand or Full, depending on if you are in the box or cursor mode:

Expand	Expand the area between the cursors.
Full	Display the full area.

The remaining buttons do not change labels:

sf wf	Opens the interactive FID windowing mode, see below.
Dscale	Toggle the display of a time scale under the FID in units specified by the `axisf` parameter.
Phase	Opens the interactive phasing mode.
Return	Returns to the last menu active before entering the `df` display.

Controlling Cursors and FID Intensity

The cursor is controlled by moving the mouse arrow and pressing the left button on the mouse. Alternatively, the left button on the mouse can be held down and the cursor tracks movement of the mouse arrow. Moving the cursor updates the parameter `crf`.

Pressing the right mouse button displays a second cursor to the right of the original cursor. Pressing the right button of the mouse (or holding the right button down) causes this new cursor to move to the mouse arrow. The second cursor may not be moved to the left of the first cursor. Movement of the second cursor updates the parameter `deltaf`, the difference in seconds between the two cursors. If both cursors are displayed, pressing the left button on the mouse enables both cursors to be moved by the same amount; this changes the parameter `crf` but not the parameter `deltaf`.

The middle mouse button controls the FID intensity. Pressing this button adjusts the vertical scale of the FID (parameter `vf`) so that the FID intensity at the position of the mouse arrow equals the vertical position of the mouse arrow. If the mouse arrow is positioned at the left edge of the display, the vertical position of the display is adjusted to the vertical position of the mouse arrow. Parameters affected are `vpfi` if the imaginary channel of the FID is displayed and `vpf` if the imaginary channel is not displayed.

After an FID is displayed with the `df` command, parameter entry updates the FID.

The left and right mouse buttons differ only in their sensitivity. Full scale (top to bottom of screen) corresponds to approximately 180° for the left button, and 20° for the right button. Therefore, consider the left button the “coarse” adjust and the right button the “fine” adjust.

During the entire phasing process, only the update region centered between the vertical cursors is redisplayed to reflect the new phase parameter. The width of this update region

is controlled by the global parameter `phasing`, which sets the percentage of the screen display to be updated:

- `phasing=20` causes only the region between the vertical cursors to be updated.
- `phasing=70` causes 70% of the screen to be updated.

The value of `phasing` can vary between 10 and 100. Continue this process until the FID in the update region is properly phased.

The middle button adjusts the vertical scale of the FID. It can also cause the latest phase correction to be applied to the entire FID. To apply this phase correction, position the mouse arrow at a point on the FID that is on-scale and click the center button. This will leave the vertical scale unaffected but will recalculate the phase of the entire FID. Clicking the center button above or below the FID will raise or lower the vertical scale.

Note that the “real” display shows the real FID (channel A) when `phfid='n'` or `0`. If `phfid=90`, the “real” display shows the imaginary FID (channel B).

Interactive FID Windowing

The sf wf button activates the interactive FID windowing mode. No cursors are displayed. The left mouse button adjusts the starting time of the displayed FID. Position the mouse arrow at some position, click the left mouse button, and a cursor is displayed at the selected time. Moving the mouse arrow to another position in the display and clicking the left mouse button drags the cursor-defined time to that new mouse arrow position.

The right mouse button adjusts the width of the displayed FID. Position the mouse arrow over some spectral region, click the right mouse button, and a horizontal and a vertical cursor intersect at the mouse arrow. Moving the mouse arrow above or below the horizontal cursor adjusts the width of the FID display. The start of the FID display is also adjusted so that the position of the displayed vertical cursor remains constant. The further the mouse arrow is moved from the horizontal cursor, the larger the size of the relative change.

Interactive Phasing Mode

The Phase button activates the interactive phasing mode:

1. Position the mouse arrow on a FID region of interest, about halfway vertically up the screen, and click the left mouse button.

   A horizontal cursor intersects at the mouse arrow and two vertical cursors are placed on either side of the mouse arrow. A small region of FID is displayed in a different color if a color display is present; only this spectral region is interactively updated.

2. Move the mouse above or below the horizontal cursor, but within the two vertical cursors. Click the left or right button to adjust the FID phase parameter `phfid`.

   Click the mouse above the horizontal cursor to increase `phfid`. Click below the horizontal cursor to decrease `phfid`. Place the mouse arrow right on the horizontal cursor and click the left button to restore the initial phase.

3. To exit the interactive phasing mode, make another selection from the menu. Select the Cursor or Box button if no other choice is desirable.

9.3 Stacked and Whitewashed FID Display and Plotting

Table 35 lists commands and parameters available for stacked and whitewashed FID display and plotting. All new parameter sets have the FID display parameters `dotflag`, `axisf`, `vpf`, `vpfi`, `crf`, and `deltaf` defined. Because old parameter sets might not have these parameters defined, the macro `addpar('fid')` is provided to create these parameters in the current experiment (the macro `fidpar` functions the same as `addpar('fid')`).

Table 35. FID Display and Plotting Commands and Parameters

Commands	
`addpar('fid')`	Add parameters for FID display in current experiment
`dfs*`	Display stacked FIDs
`dfsa*`	Display stacked FIDs automatically
`dfsan*`	Display stacked FIDs automatically without screen erase
`dfsh*`	Display stacked FIDs horizontally
`dfshn*`	Display stacked FIDs horizontally without erasing screen
`dfsn*`	Display stacked FIDs without erasing screen
`dfww*`	Display FIDs in whitewash mode
`fidpar`	Add parameters for FID display in current experiment
`pfww*`	Plot FIDs in whitewash mode
`plfid*`	Plot FIDs
`* dfs<(<start><,finish><,step><,'all'|'imag'><,color>)>`	
`dfsa<(<start><,finish><,step><,'all'|'imag'><,color>)>`	
`dfsan<(<start><,finish><,step><,'all'|'imag'><,color>)>`	
`dfsh<(<start><,finish><,step><,'all'|'imag'><,color>)>`	
`dfshn<(<start><,finish><,step><,'all'|'imag'><,color>)>`	
`dfsn<(<start><,finish><,step><,'all'|'imag'><,color>)>`	
`dfww<(<start><,finish><,step><,'all'|'imag'><,color>)>`	
`pfww<(<start><,finish><,step><,'all'|'imag'>)>`	
`plfid<(<start><,finish><,step><,'all'|'imag'><,pen>)>`	
Parameters	
`axisf` {'s','m','u','n'}	Axis label for FID displays and plots
`crf` {number, in sec}	Current time-domain cursor position
`deltaf` {number, in sec}	Difference of two time cursors
`dotflag` {'n','y'}	Display FID as connected dots
`ho` {number, in mm}	Horizontal offset
`lsfid` {'n', number}	Number of complex points to left-shift np FID
`phfid` {'n',–360 to 360, in deg}	Zero-order phasing for np FID
`sc` {0 to wcmax, in mm}	Start of chart
`sf` {0 to at, in sec}	Start of FID display
`vf` {1e–6 to 1e9}	Vertical scale of FID
`vo` {number, in mm}	Vertical offset
`vpf` {number, in mm}	Current vertical position of FID
`vpfi` {number, in mm}	Current vertical position of imaginary FID
`wc` {5 to wcmax, in mm}	Width of chart
`wf` {0 to at, in sec}	Width of FID plot

Stacked FIDs

The `dfs` command displays one or more FIDs as a *stacked display* in which each FID is offset horizontally and vertically from the previous FID. The position of the first FID is governed by the parameters `wc`, `sc`, and `vpf`. Each subsequent FID is positioned relative

to the preceding FID by the offset parameters vo and ho. For a "left-to-right" presentation, ho is usually negative; for a "bottom-to-top" presentation, vo is positive. The syntax for dfs is the following:

```
dfs<(<start><,finish><,step><,'all'|'imag'><,color>)>
```

For arrayed 1D or 2D data sets, a particular FID can be viewed by supplying the index number as an argument. Multiple FIDs can be displayed by supplying the indices of the first and last FIDs. The optional step argument is the increment for the FID index (the default is 1). If 'imag' is supplied as a keyword argument, only the imaginary FID channel is displayed (the default is 'all', to display all FIDs). A color ('red', 'green', 'blue', etc.) can be supplied as an argument as well.

The following commands are variations of dfs and use the same arguments as dfs:

- dfsn functions the same as dfs except the graphics screen is not erased before the display starts. This allows composite displays of many FIDs to be created.
- dfsa displays one or more FIDs automatically by adjusting the parameters vo and ho to fill the screen in a lower left to upper right presentation (wc must be set to less than full screen width for this to work). The position of the first FID is governed by parameters wc, sc, and vpf.
- dfsan functions the same as dfsa except the graphics screen is not erased before the display starts. This allows the creation of composite displays of many FIDs.
- dfsh displays one or more FIDs horizontally by setting vo to zero and adjusting ho, sc, and wc to fill the screen from left to right with the entire array. The position of the first FID is governed by parameters wc, sc, and vpf.
- dfshn functions the same as dfsh except the graphics screen is not erased before the display starts. This allows composite displays of many FIDs to be created.

The plfid command plots one or more FIDs as a stacked display. This command uses the same arguments as dfs and functions the same as dfs except, instead of displaying FIDs, plfid plots the FIDs, and instead of a screen color, plfid can be supplied with a pen number ('pen1', 'pen2', 'pen3', etc.) as an optional argument.

Whitewashed FIDs

The dfww command displays *whitewashed FIDs*—a display in which FIDs after the first ones are blanked out in regions in which they are behind the earlier FIDs. Other than the difference in displays, dfww and dfs function the same and use the same arguments.

The pfww command plots whitewashed FIDs. This command functions the same as dfww except that pfww plots FIDs and does not use the color argument.

9.4 Interactive Spectrum Display

After data is transformed, a spectrum becomes available for display and plotting. The normal spectrum display program is ds, which enables interactive manipulation of a single 1D spectrum. ds is entered by the command ds<(index)> or from the menu system by selecting one of the buttons Transform or Weight,Transform in the 1D Data Processing Menu. Table 36 lists commands and parameters associated with the interactive spectra display.

Table 36. Interactive Spectrum Display Commands and Parameters

Commands	
`cz<(freq1,freq2,...)>`	Clear integral reset points
`ds<(index)>, ds<(options)>`	Display a spectrum
`inset`	Display an inset spectrum
Parameters	
`cr` {number}	Current cursor position
`delta` {number, in Hz}	Difference of two frequency cursors
`intmod` {'off', 'full', 'partial'}	Integral display mode
`io` {0 to 200, in mm}	Integral offset
`is` {1 to 1e9}	Integral scale
`lp` {–3600 to +3600, in deg.}	First-order phase on directly detected dimension
`lvl` {number}	Zero-order baseline correction
`lvltlt` {number}	Control sensitivity of `lvl` and `tlt` adjustments
`phasing` {10 to 100, in %}	Control update region during interactive phasing
`rp` {–360 to +360, in deg.}	Zero-order phase on directly detected dimension
`tlt` {number}	First-order baseline correction
`vp` {–200 to +200, in mm}	Vertical position of spectrum
`vs` {1e–6 to 1e9}	Vertical scale

Interactive 1D Spectrum Display Menus

Upon entry to `ds`, the screen contains a spectrum similar to Figure 67.

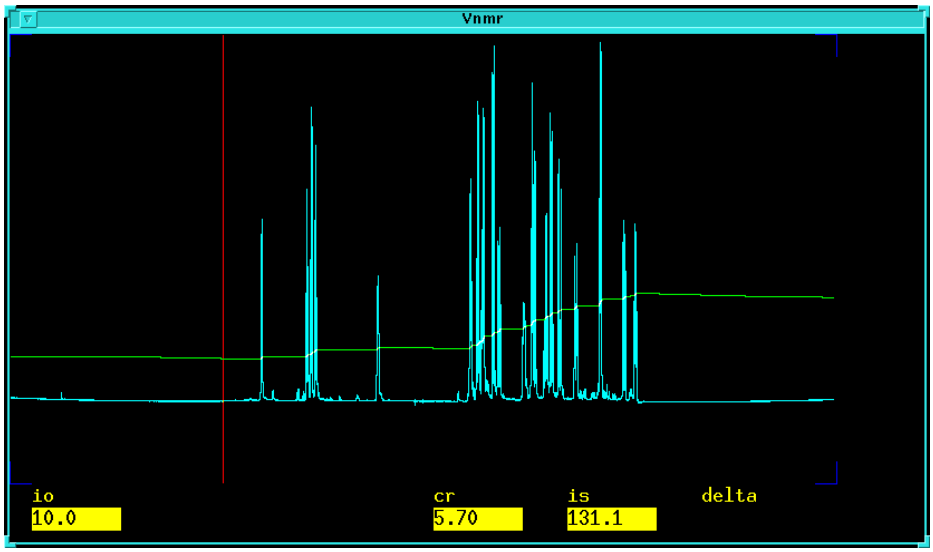


Figure 67. Interactive Spectrum Display (`ds` program)

At the top of the display is the Interactive 1D Spectrum Display Menu with the following buttons (the labels change on some of the buttons according to the mode the program is in):

The buttons on the Interactive 1D Spectrum Display Menu function as follows:

The first button is Box or Cursor, depending on if you are in the box or cursor mode:

Box	Change to the box mode with two cursors.
Cursor	Change to the cursor mode with one cursor.

The second button is No Integral, Full Integral, or Part Integral, depending on which integral display mode you are in:

No Integral	Hide the integral display.
Full Integral	Display all integral regions.
Part Integral	Display every other region.

The third button is Expand or Full, depending on if you are in the box or cursor mode:

Expand	Expand spectral region between cursors to the full width of chart.
Full	Set displayed spectrum to its full spectral width.

The remaining buttons do not change labels:

sp wp	Open an interactive spectral windowing mode, described below.
Mark	If selected in the cursor mode, the position and spectral intensity at that point are displayed and written into a file `mark1d.out` in the current experiment directory file (e.g., `/home/vnmr1/vnmrsys/exp2/mark1d.out`). If selected in the box mode, the values of both cursor positions, the spectral intensity of the maximum between the cursors, and the total integral between the cursors are displayed and written into the file.
Phase	Open an interactive phasing mode, described below.
Th	Toggles the display of a horizontal cursor. The left mouse button positions this cursor at the mouse arrow position. The middle mouse button adjusts the scale, as described below.
resets	Open an interactive integral reset mode, see below.
Dscale	Toggle on and off the display of a scale below the spectrum.
Lvl/Tlt	Open interactive zero- and first-order baseline correction mode, see below.
Set Int	Set the value of an integral.
Ref	Set spectral referencing.
Return	Return to the last menu active before entering `ds`.

Controlling the Cursors and Spectral Intensity

The cursor is controlled by moving the mouse arrow and pressing the left mouse button. Alternatively, the left mouse button can be held down and the cursor will track any movement of the mouse arrow. The parameter `cr` is updated by movement of this cursor.

Pressing the right mouse button will display a second cursor to the right of the original cursor. Subsequent depression of the right mouse button (or holding the right button down) will cause this new cursor to move to the mouse arrow. The parameter `delta` will be updated by movement of this second cursor. This second cursor may not be moved to the left of the first cursor. If both cursors are displayed, depression of the left mouse button enables both cursors to be moved by the same amount. That is, the parameter `cr` is changed but the parameter `delta` is not changed.

The middle mouse button controls the spectral intensity. Pressing this button causes the vertical scale of the spectrum (parameter `vs`) to be adjusted so that the spectral intensity at the position of the mouse arrow equals the vertical position of the mouse arrow. If an optional integral is displayed when the middle mouse button is depressed, the integral scale (parameter `is`) will be adjusted so that the integral intensity at the position of the mouse arrow equals the vertical position of the mouse arrow. If the mouse arrow is positioned at

the left edge of the display, the vertical position of the display will be adjusted to the vertical position of the mouse arrow. The parameter affected will be `io` if the integral is displayed or `vp` if the integral is not displayed.

Interactive Spectral Windowing Mode

The sp wp button activates interactive spectral windowing mode. No cursors will be displayed. The left mouse button is used to adjust the starting frequency of the displayed spectrum. Position the mouse arrow at some position and click the left mouse button. A cursor will be displayed at the selected frequency. Moving the mouse arrow to another position in the display and clicking the left mouse button will "drag" the cursor defined frequency to that new mouse arrow position.

The right mouse button is used to adjust the width of the displayed spectrum. Position the mouse arrow over some spectral region and click the right mouse button. A horizontal and a vertical cursor will intersect at the mouse arrow. Moving the mouse arrow above or below the horizontal cursor will adjust width of the spectral display. The start of the spectral display will also be adjusted so that the position of the displayed vertical cursor remains constant. The further the mouse arrow is from the horizontal cursor, the larger the size of the relative change.

Interactive Phasing Mode

The Phase button starts the interactive phasing mode. Any integral and cursors that are displayed along with the spectrum are removed.

Position the mouse arrow on a spectral region of interest toward the right side of the spectrum, about halfway vertically up the screen, and click the left mouse button. A horizontal cursor will intersect at the mouse arrow. Two vertical cursors will be placed on either side of the mouse arrow. A small region of the spectrum will be displayed in a different color, if a color display is present, and only this spectral region will be interactively updated. Now moving the mouse above or below the horizontal cursor, but within the two vertical cursors, and clicking the left or right button will adjust the zero-order or frequency-independent phase parameter `rp`. Clicking the mouse above the horizontal cursor will increase `rp` (cause a clockwise rotation of the peaks), while clicking below the horizontal cursor will decrease `rp` (and cause a counter-clockwise rotation). Placing the mouse arrow right on the horizontal cursor and clicking the left button will restore the initial phase.

The left and right button of the mouse differ only in their sensitivity. Full scale (top to bottom of the screen) corresponds to approximately 180° for the left button, and 20° for the right button, and hence you can consider the left button the "coarse" adjust and the right button the "fine" adjust.

During this entire process, only the update region centered between the vertical cursors will be redisplayed to reflect the new phase parameter. The width of this update region is controlled by the global parameter `phasing`, which sets the percentage of the screen display to be updated. `phasing=20` will cause only 20% of the screen to be updated; `phasing=70` will cause 70% of the screen to be updated. The value of `phasing` can vary between 10 and 100. Continue this process until the peak or peaks in the update region are properly phased.

Now move the mouse arrow to another region of the spectrum, near the left edge of the display, outside the vertical cursors, and click the left mouse button again. The frequency-independent phase-correction made so far will first be applied to the entire spectrum. A new horizontal cursor will be displayed at the mouse arrow, and two new vertical cursors will

be displayed on either side of the mouse arrows. The mouse will now control the first-order or frequency-dependent phase parameter `lp`. Clicking the left or right button above or below the horizontal cursor will now increase or decrease `lp`, and will also change `rp` so that the phase at the center of the previous region bracketed by the vertical cursors will be held constant. This process eliminates or substantially reduces the necessity to iteratively adjust the two parameters `rp` and `lp`. As with the zero-order correction, the left button acts as a “coarse” adjust, and the right button as a “fine.”

Each time the mouse arrow is moved outside of the two vertical cursors and the mouse button is clicked, a new update region is defined below the mouse arrow and new horizontal and vertical cursors are displayed. Subsequent first-order phase changes causes the zero-order phase to be adjusted such that the phase angle at the center of the previous region bracketed by the vertical cursors remains constant. If you wish to return to the zero-order phase correction, the Phase button in the menu must be reselected.

The middle mouse button adjusts the vertical scale of the spectrum. In addition, it causes the latest phase correction to be applied to the entire spectrum. To do this, position the mouse arrow at the very top of a peak that is on scale, and click the center button. This leaves the vertical scale unaffected but recalculates the phase of the entire spectrum. Clicking the center button above or below the peak raises or lowers the vertical scale.

To exit the interactive phasing mode, make another selection from the menu; the first button (Cursor or Box) is always an appropriate choice if no other choice is desirable.

Interactive Integral Reset Mode

The resets button activates the interactive integral reset mode. No cursors are displayed. The left mouse button defines an integral reset at the current mouse arrow position. The right mouse button removes an integral reset closest to the current mouse arrow position. The middle mouse button adjusts the scale, as described above.

The integral does not have to be displayed. However, if the integral is displayed in the “partial” mode, the normally blanked regions are displayed as dotted lines. To clear the integral reset points before beginning, the command `cz` must be used; no menu choice is provided for this action.

Interactive Zero- and First-Order Base Correction Mode

The Lvl/Tlt button activates interactive zero and first order baseline correction mode. The zero order correction is represented by the `lvl` parameter; the first order correction is represented by the `tlt` parameter. If no integral is displayed when the lvl/tlt button is activated, the integral is automatically displayed.

Position the mouse arrow on an integral region of interest, about halfway vertically up the screen, and click the left mouse button. A horizontal cursor will intersect at the mouse arrow. Two vertical cursors will be placed on either side of the mouse arrow. Now moving the mouse arrow above or below the horizontal cursor, but within the two vertical cursors, and clicking the left or right button will adjust the zero-order baseline correction parameter `lvl`. Clicking the mouse above the horizontal cursor will increase `lvl`, while clicking below the horizontal cursor will decrease `lvl`. Placing the mouse arrow right on the horizontal cursor and clicking the mouse button will restore the initial baseline correction value.

Now move the mouse arrow to another region of the spectrum, outside the vertical cursors, and click the left mouse button again. A new horizontal cursor will be displayed at the mouse arrow, two new vertical cursors will be displayed on either side of the mouse arrow,

and a single vertical cursor will be displayed in the middle of the region where `lvl` was being updated. The mouse will now control the first-order baseline correction parameter `tlt`. Clicking the left or right mouse button above or below the horizontal cursor will now increase or decrease `tlt`, and will also change `lvl` so that the total drift correction at the single vertical cursor in the middle of the previous region will be held constant. This process eliminates or substantially reduces the necessity to iteratively adjust the two parameters `lvl` and `tlt`. As with the zero-order correction, placing the mouse arrow right on the horizontal cursor and clicking the mouse button will restore the initial baseline correction values.

Each time the mouse arrow is moved outside the two vertical cursors and the mouse button is clicked, a new vertical and horizontal cursor is displayed. The parameter adjustment alternates between adjusting only the `lvl` parameter and adjusting both the `lvl` and `tlt` parameters.

The left and right mouse buttons both adjust the baseline correction parameters and differ only in their sensitivity. The left button causes changes a factor of eight times larger than the right button, and hence you can consider the left button the “coarse” adjust and the right button the “fine” adjust. The overall sensitivity of these adjustments can also be controlled by the parameter `lvltlt`. This parameter is a multiplier, with a default value of 1.0, for the size of the changes. To make larger changes, make `lvltlt` larger than 1.0. To have finer control, set `lvltlt` to be between 0.0 and 1.0.

The middle mouse button adjusts the integral scale (parameter `is`) or the integral offset (parameter `io`), exactly as whenever an integral is displayed.

To exit the interactive baseline correction mode, make another selection from the menu; the first button (Cursor or Box) is always an appropriate choice if no other choice is desirable.

Setting the Integral Value

1. Position a cursor over an integral region, and then press the Set Int button to display:
   `Current integral is xx. New value?`
2. Enter the value you want to assign to that integral region.

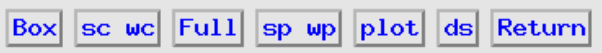
Setting the Reference Position

1. Position a cursor on the reference line, and then press the Ref button to display:
   `New reference value (in ppm)?`
2. Enter the value you want to assign to that line.

Interactive Inset Display

The `inset` command displays the part of the spectrum between the two cursors in `ds` as an inset. The vertical position of the `inset` spectrum is shifted up about one-quarter of the height of the whole display window. The old spectrum remains on the screen, but the parameters shown at the bottom are now relevant to the inset display. If present, the integral trace and the scale are duplicated with the `inset` spectrum.

After running `inset`, you can shift the displayed spectrum, expand it, or even contract it with the left and right mouse buttons and the following menu (notice that the labels change on some of the buttons according to the mode the program is in):



These buttons function as follows:

The first button is Box or Cursor, depending on if you are in box or cursor mode:

Box	Change to the box mode with two cursors.
Cursor	Change to the cursor mode with one cursor.

The second button does not change labels:

sc wc	Interactively adjust start of the display and its width on the screen.

The third button is Expand or Full, depending on if you are in the box or cursor mode:

Expand	Expand the area between the cursors.
Full	Display the full area.

The remaining buttons do not change labels:

sp wp	Interactively adjust the starting frequency and width of frequencies displayed in the spectrum
plot	Plot the spectrum, and if displayed, the integral and the scale.
ds	Return to the `ds` menu without erasing the display.
Return	Return to the 1D Display Menu.

While working with the `inset` display, the mouse buttons function as follows:

- The left mouse button positions the cursor or pair of cursors. In the sc wc mode, the left button adjusts the starting position of the display. In the sp wp mode, the left button adjusts the starting frequency in the display.
- The center mouse button changes the vertical scale of the spectrum or integral so that it goes through the current mouse position. If the mouse cursor is positioned at the left edge of the spectrum, the horizontal position of the spectrum or integral is adjusted.
- The right mouse button positions the second cursor relative to the first cursor. In the sc wc mode, the right button adjusts the width of the display on the screen. In the sp wp mode, the right button adjusts the width of frequencies displayed.

9.5 Spectral Display and Plotting

Table 37 lists spectral display commands and parameters, and Table 38 lists commands primarily associated with plotting of spectra.

The two tables work together. The tools in Table 37 are used to set up the spectra on the screen for plotting using the tools in Table 38.

Display Parameters

Parameters intended mostly for spectral display include `vs`, `sp`, `wp`, `vp`, `cutoff`, `th`, `axis`, `rfp`, and `rfl`. The `s`, `fr`, and `r` macros allow working with the display parameters as a set:

- The `s` macro saves a copy of the current values of all display parameters as a display parameter set. Up to nine sets can be saved, with the labels set 1, set, 2, etc. The `s` command is entered as `s#`, where # is the number from 1 to 9 of the display parameter set, (e.g., entering `s3` saves set 3).
- The `fr` macro, entered as `fr#`, where # ranges from 1 to 9 (e.g., `fr3`), performs a full recall of display parameter set #, setting current display parameters to those values.
- The `r` macro, entered as `r#`, where # ranges from 1 to 9 (e.g., `r3`), recalls most of display parameter set # except phase parameters, drift correction parameters, integral reset parameters, and reference parameters.

Table 37. Spectral Display Commands and Parameters

Commands	
`ai`	Select absolute intensity mode
`center`	Set display limits for center of screen
`crl`	Clear reference line
`dll*`	Display listed line frequencies and intensities
`dpf*`	Display peak frequencies over spectrum
`dres*`	Measure linewidth and digital resolution
`dscale*`	Display scale below spectrum or FID
`dtext<(file,x,y)><:xn,yn,inc>`	Display a text file in the graphics window
`f`	Set display parameters to full spectrum
`frset_number, fr(set_number)`	Full recall of a display parameter set
`full`	Set display limits for a full screen
`left`	Set display limits to left half of screen
`nl<:height<,frequency>>`	Position cursor at nearest line
`nm`	Select normalized intensity mode
`noislm<(max_noise)>`	Adjust vertical scale to limit noise level
`rset_number, r(set_number)`	Recall display parameter set
`right`	Set display limits to right half of screen
`rl<(frequency)>`	Set reference line
`sset_number, s(set_number)`	Save display parameters as a set
`setref*`	Set frequency referencing for proton spectra
`setoffset(nucleus,ppm):offset`	Calculate offset frequency for given nucleus and ppm
`split`	Split difference between two cursors
`thadj*`	Adjust threshold for peak printout
`tmsref:tms_found`	Reference spectrum to TMS
`vsadj<(height)>`	Adjust vertical scale
`vsadj2<(height)>:factor`	Adjust vertical scale in powers of two
`vsadjc<(height)>`	Adjust vertical scale of carbon spectra
`vsadjh<(height<,do_not_ignore)>`	Adjust vertical scale of proton spectra
`zoom(width)`	Adjust display to given width

```
* dll<('pos'<,noise_mult>)><:number_lines,scale>
  dpf<(<'noll'><,'pos'><,noise_mult><,'leader'><,length>)>
  dres<(<freq<,fractional_height>>)>:linewidth,digital_resolution
  dscale<(<axis><,vertical_start><,display_start><,color>)>
  setref<(nucleus)>:$rfl,$rfp,$reffrq,$refpos
  thadj<(maximum_peaks<,noise_mult<,llarg1<,llarg2>>>)>
```

Parameters	
`aig` {'ai','nm'}	Absolute intensity group
`axis` {'h','p','k'}	1D axis label for displays and plots
`cutoff` {number, in mm}	Data truncation limit
`cutoff` {number, in mm}	Data truncation limit
`dmg` {'ph','av','pwr', 'pa'}	Data display mode, directly detected dimension
`rfl` {number, in Hz}	Reference peak position
`rfp` {number, in Hz}	Reference peak frequency
`th` {0 to 1e9, in mm}	Threshold
`vp` {–200 to +200, in mm}	Vertical position of spectrum
`vs` {1e–6 to 1e9}	Vertical scale
`wysiwyg` {'y','n'}	Set plot display or full display

Table 38. Spectral Plotting Commands and Parameters

Commands	
`aexppl<(expansion_factor)>`	Automatic plot of spectral expansion
`pl*`	Plot spectra
`plc<(pltmod)>`	Plot carbon spectrum
`plh<(pltmod)>`	Plot proton spectrum
`pll<(x,y,minimum_y)>`	Plot a line list
`plp<(pltmod)>`	Plot phosphorus spectrum
`plot`	Automatically plot spectra
`plot1d`	Plotting macro for simple (non-arrayed) 1D spectra
`ppf*`	Plot peak frequencies over spectrum
`pscale*`	Plot scale below spectrum or FID
`* pl<(<start,finish,step><,'int'><,'all'><,options>)>`	
`ppf<(<'noll'><,'pos'><,noise_mult><,'top'>)>,`	
`ppf<(<'noll'><,'pos'><,noise_mult><,'leader'><,length>)>`	
`pscale<(<'fid'><,axis><,vertical_start><,plot_start><,pen>)>`	
Parameters	
`hzmm` {number}	Scaling factor for plots
`pltmod*`	Plotter display mode
`sp` {number, in Hz}	Start of plot
`wp` {number, in Hz}	Width of plot
`* pltmod` {'off','fixed','full','standard','user','variable'}	

The vertical position (in mm) of the spectrum with respect to the bottom of the display is set by the `vp` parameter. The `cutoff` parameter defines the distance above and below the current vertical position at which the spectrum is truncated. For example, `cutoff=50` will truncate data at `vp+50` mm and `vp-50` mm.

Vertical Scale Adjustment

Two vertical scaling modes are available, normalized and absolute intensity:

- The `nm` command selects the *normalized display mode* in which spectra are scaled so that the largest peak in the spectrum is `vs` mm high.
- The `ai` command selects the *absolute-intensity mode* in which the scale is kept constant from spectrum to spectrum. This allows comparison of peak heights from one spectrum to another.

The modes are mutually exclusive— the system is always either in normalized or absolute-intensity display mode. The `aig` parameter contains the result of the `ai` or `nm` command. It can be queried (`aig?`) to determine which display mode is active.

The `vsadj` macro automatically sets the vertical scale adjustment `vs` in the `ai` mode so that the largest peak is `0.9*(wc2max-vp-sc2)` mm tall. The syntax is `vsadj<(height)>`. Include `height` as an argument to specify the desired height, in mm, of the largest signal in the displayed portion of the spectrum.

The macros `vsadjh` and `vsadjc` function the same as `vsadj` except that the solvent and TMS signals are disregarded from their respective proton or carbon spectra for the vertical scale adjustment. `vsadjh` also has the `do_not_ignore _solvent` argument that changes `vsadjh` actions to include the solvent line and to exclude only the TMS line.

The `vsadj2` macro adjusts the vertical scale by powers of two as required for expansion plots. The syntax is `vsadj2<(height)>:scaling_factor`. The argument

`height` is used the same as in `vsadj`. `scaling_factor` returns the ratio of the new compared to the old value of `vs` to the user or the calling macro.

The `noislm` macro limits the noise present in a spectrum by reducing the vertical scale `vs`. If the noise is smaller than the noise limit, `vs` is left untouched. The noise limit is in single root-mean-square noise size; the peak-to-peak noise (width of the noise band) is about twice that value. The noise is determined by taking the smallest value from four 5% regions at the left end of the spectrum. Any filter cutoff at the end will decrease the apparent noise in the spectrum, and therefore increase the noise limit in the central part of the spectrum. Because of the particular algorithm used in this macro, signals at the left end of the spectrum should not affect the result of `noislm`. An optional argument, `max_noise`, can be entered to `noislm`. `max_noise` is the maximum root-mean-square size, in mm, of the noise (the default is 2).

Line Listings

The `nl` command moves displayed cursor to nearest line and displays its height and frequency (in Hz and ppm).

The `dll` command displays line frequencies and intensities that are above a threshold defined by the parameter `th`. The number of lines and a scaling factor for line amplitudes can be returned to the caller. The list of line frequencies above `th` is stored by the `llfrq` parameter. Frequency units are defined by the parameter `axis`. Frequencies are stored in Hz and are not adjusted by parameters `rfl` and `rfp`. The argument `noise_mult` to `dll` enables suppressing noise peaks. The default value of `noise_mult` is 3. A smaller value results in more peaks, a larger value results in fewer peaks, and a value of 0.0 results in a line listing containing all peaks above `th`. The list of line amplitudes above `th` is stored by the `llamp` parameter. Amplitudes are stored as the actual data point value; they are not scaled by `vs`.

The `thadj` command adjusts the threshold `th` to select peaks. The syntax is
`thadj<(maximum_peaks<,noise_mult<,llarg1<,llarg2>>>)>`

where, the `maximum_peaks` specifies the maximum number of peaks desired above the threshold (the default is `wc`/4), `noise_mult` is a noise multiplier used to calculate the minimum value for `th` from the size of the root-mean-square noise (the default is 3), and `llarg1` and `llarg2` are arguments for the `noise_mult` and a keyword, respectively, sent to the `nll` command used inside `thadj`.

The `dpf` command displays peak frequencies, in units specified by the `axis` parameter, on the graphics screen, selecting only those peaks greater than `th` high. Among the options for `dpf` are `'noll'`, `'pos'`, and `noise_mult.` The command `dpf('noll')` displays peak frequencies using the last previous line listing and `dpf('pos')` displays positive peaks only. Any subsequent changes in the display will require a new `ds` command to erase the displayed frequencies. The `noise_mult` argument suppresses noise peaks and uses the same values as given for the `dll` command above. Control of label position is available through the optional `'leader'`, `'top'`, and `length` arguments.

The `dscale` command displays a scale under the spectrum or FID. The syntax is
`dscale<(<axis><,vert_start><,display_start><,color>)>`

where `axis` specifies the units, `vertical_start` is the vertical position, `display_start` modifies the start of the plot, and `color` is the color of the scale.

Line Resolution

The `dres` command displays the resolution of a line, as well as the limiting digital resolution of the spectrum, selected by the displayed cursor. The resolution is determined by a width at half-height algorithm and not by least-squares.

Referencing

VNMR frequency referencing is based on a number of parameters:

`rfl`	*Reference line* – The distance of the reference line from the right edge of the spectral window. This line is the spectral position used to set the referencing. It can be the signal of a frequency standard (such as TMS), or any line (such as a solvent signal) with a known chemical shift (in ppm), or a position in the spectrum where you expect such a line to appear.
`rfp`	*Reference position* – The difference between the reference line and the reference frequency (zero position of the scale), in Hz. If you reference a spectrum using the signal of a frequency standard, such as TMS, then `rfp` is 0. The distance of the reference frequency from the right edge of the spectrum is `rfl - rfp`.
`sfrq`	*Spectrometer frequency* – The absolute frequency, in MHz, of the center of the spectrum (the transmitter position). In order to see the accurate value of the `sfrq` parameter, you should use the `spcfrq` command.
`reffrq`	*Reference frequency* – The frequency, in MHz, of the frequency standard, i.e., the zero position of the frequency scale, *and* the divider (unit) for the calculation of ppm scales.
`refpos`	Used only for internal housekeeping and is normally set to zero. It also indicates whether the referencing is used (on) or not (`refpos='n'`).

The `rl` command is used to reference a spectrum based on the current cursor position. If you want to reference the spectrum based on a line position in the spectrum, first use the `nl` command to place the cursor at the exact position of that line. If no argument is given, `rl` defines the current cursor position as the reference frequency:

```
reffrq = sfrq + (cr + rfl - sw/2)/1e6
```

At the same time, `rfl` is set to the distance of the cursor from the right edge of the spectrum, in Hz:

```
rfl = sw/2 - (sfrq - reffrq)*1e6
```

and the parameter `rfp` is set to 0, because we have referenced the spectrum based on the position of the reference frequency itself.

Optionally, `rl` takes the position of the reference line, in Hz, as an argument. For example, if you reference a proton spectrum to the chloroform ($CHCl_3$) solvent line, you would position the cursor on that signal and enter `nl rl(7.24p)`. `rl` first calculates the absolute cursor position as

```
absolute_cr = sfrq + (cr + rfl - rfp - sw/2)/1e6
```

and can then calculate `reffrq` as

```
reffrq = (1/(1 + (argument_1/reffrq)/1e6))*absolute_cr
```

`refpos` is set to 0, `rfl` and `rfp` are calculated as follows:

```
rfl = sw/2 + (absolute_cr - sfrq)*1e6
rfp = (absolute_cr - reffrq)*1e6
```

The `crl` command clears the reference line by removing any spectral referencing present. It also sets `refpos='n'` (turns off referencing). After this operation, zero frequency appears at the right edge of the spectrum.

The `tmsref` command tries to locate a TMS line. If found, `tmsref` re-references the spectrum to the TMS line and returns a 1 to the calling macro; if not found, `tmsref` returns 0 and the referencing is left as it was. In the case of other signals (e.g., from silicon grease) immediately to the left of the TMS line (even if they are higher than the reference line), `tmsref` tries avoiding those by taking the line furthest to the right in that area, as long as it is at least 10% of the main Si-CH_3 signal. Large signals within 0.6 ppm for ^{1}H (or 6 ppm for ^{13}C) to the right of TMS may lead to misreferencing

The `setref` macro adjusts the referencing so that the solvent frequency is correct. Even when no reference substance is present in the sample, `setref` uses absolute resonance frequencies (calculated for a proton frequency of 100.0000000 MHz) as defined in the file `/vnmr/nuctables/nuctabref`, which contains about 25 of the most common nuclei. `setref` can easily be expanded to cover any other nucleus as well; a recipe on how to expand `setref` is given in the header of the file `/vnmr/nuctables/nuctabref`.

The `setref` macro assumes that the system is locked (and that the lock solvent is defined in `/vnmr/solvents`). If you are working without lock and still want to use `setref`, you must ensure that the field offset has been previously adjusted so that the lock frequency is on resonance with a sample of similar susceptibility. To ensure that the field offset is adjusted, do the following procedure:

1. Insert a sample with deuterated solvent.
2. Adjust `z0` (or `lkof`) in `acqi` so that the lock frequency is on resonance.
3. Switch off the lock.
4. Insert the nondeuterated sample.

On UNITY*INOVA* systems, `setref` first calculates the lock frequency, in MHz, as
`lock_frequency` `= lockfreq + lkof/1e6`

For most other systems, the lock frequency is equal to `lockfreq`, except for UNITY and VXR-S systems, where it must be calculated from `lockfreq`.

`setref` can calculate the deuterium reference frequency, based on the chemical shift of the ^{2}H lock signal (*`lock_shift`*), which is extracted from the file `/vnmr/solvents` using the `solvinfo` command:
`h2_ref` `=` *`lock_frequency`*`/(1 +` *`lock_shift`*`/1e6)`

This is the frequency of the deuterium frequency standard (0 ppm) at the current field strength. Using the ratio of the absolute (standard) resonance frequencies for deuterium (*`stdfrq_h2`*) and for the current nucleus (*`stdfrq_tn`*), the `reffrq` parameter can now be calculated directly:
`reffrq =` *`h2_ref*stdfrq_tn/stdfrq_h2`*

Now, `rfl` can be calculated as
`rfl = sw/2 - (sfrq - reffrq)*1e6`

`rfp` is set to 0 (referencing on the frequency standard), and `refpos` is set to 0 (referencing active). `setref` returns the values of `rfl`, `rfp`, `reffrq`, and `refpos` to the calling macro.

The accuracy of the `setref` macro is mostly limited by the accuracy of the chemical shift of the lock resonance line, which may depend on the concentration and the chemical properties (acidity/basicity) of the components in the sample. But `setref` should

normally be accurate enough for macros such as `tmsref` to find an actual reference line close to its predicted position.

`setref` assumes a locked sample; however. It is possible to also use `setref` to preestimate the position if the reference frequency in spectra from unlocked samples, provided the spectrometer is first locked on a sample with similar susceptibility, then (in `acqi`) the lock is disengaged and the field offset adjusted such that the lock signal is on-resonance. Now, you can acquire spectra without lock and calculate their (estimated) referencing using `setref`, provided the `solvent` parameter is set to the solvent the system was last locked on.

The `setoffset` macro uses `setref` to calculate offset frequency for a chemical shift

The macros `setref1` and `setref2` are used to reference f_1 and f_2 in multidimensional spectra, respectively. They take the "frequency-relevant" nucleus as argument (`tn` for homonuclear nD spectra, `dn` for f_1 in heteronuclear 2D spectra, etc.), and both call `setref` (with that nucleus as argument) for the calculation of the referencing parameters.

Spectral Plotting

The `pl` command plots the currently displayed region of the currently active spectrum, or spectrum plus integral (or the region which `would` be displayed if there were a spectral display on the screen). `pl('int')` plots the integral only. `pl('pen2')` plots the spectrum using pen number 2 of a multi-pen plotter.

The `pscale` command plots a scale under a spectrum. The syntax is
`pscale<(<axis><,vertical_start><,plot_start><,pen>)>`

If the letter `p`, `h`, `k`, etc. is supplied as an optional argument for `axis`, that is used instead of the current value of the parameter `axis`. The optional argument `vertical_start` defines the vertical position where the scale is drawn (the default is 5 mm below the current value of the parameter `vp`). The second optional argument `plot_start` is interpreted as a modified start of plot. The `pen` option defines the pen number to be used.

The `ppf` command plots peak frequencies, in units specified by the `axis` parameter, above the peaks, selecting only those peaks greater than `th` high. `ppf('noll')` plots peak frequencies using the last previous line listing while `ppf('pos')` plots positive peaks only. Other arguments for noise suppression (`noise_mult`) and label positioning work the same as the `dpf` command, described above.

The `pll` command produces a columnar line list on a plotter, similar to what would appear on a printer. The output is automatically formatted into multiple columns, depending on the number of lines. The syntax is `pll<(x,y,minimum_y)>`. The arguments `x` and `y` are the *x* and y position of the upper left of the line list, and `minimum_y` is the minimum *y* at which to reset back to the top.

The `plh` command plots a proton spectrum based on parameters `pltmod` and `intmod`:

- `pltmod='off'` sets no plotting.
- `pltmod='fixed'` takes `sp` and `wp` as is.
- `pltmod='full'` adjusts `sp` and `wp` to plot the full spectrum.
- `pltmod='standard'` uses a macro that adapts output for a variety of spectra.
- `pltmod='user'` executes a user macro named `userplh`.
- `pltmod='variable'` adjusts `sp` and `wp` to plot only the region of interest.
- `intmod='off'` gives no integral.
- `intmod='partial'` gives a series of integrals over each region.

- `intmod='full'` gives a single integral over the entire spectrum.

Similarly, `plc` plots a carbon spectrum and `plp` plots a phosphorus spectrum based on the parameters `pltmod` and `intmod`, as described above. For both macros, the user macro is `userplc` if `pltmod='user'`.

Given a spectrum divided into regions by the `region` command or by the cursors in the `ds` program, the macro `aexppl<(expansion_factor)>` plots automatically each region at the horizontal scale requested (in Hz/mm). The default scale is 2 Hz/mm.

Several generic plotting macros, such as `plot` and `plot1d`, are available that call specialized plotting macros, depending on the user definition or other wise on the type of data in the experiment. For details, see the *VNMR Command and Parameter Reference*.

Display Limits

Because of the use of different plotters with different dimensions, the parameters `sc`, `wc`, `sc2`, and `wc2` need to be set differently to position plots and displays in the same *relative* position on the page. The `full`, `center`, `left`, and `right` commands do nothing more than modify `sc`, `wc`, `sc2`, and `wc2` to place the display and plot in the desired portion of the screen and page. The `f` command is used to set the `sp` and `wp` parameters to display a full spectrum. The `zoom(width)` macro adjusts the display limits to the width specified, in Hz, setting the limits to ±`width/2`. Also available is the `split` macro, which repositions the left-hand cursor halfway between its original position and the position of the left cursor.

A scaling factor helpful for 1D plotting is the `hzmm` parameter, which contains the quotient of `wp` divided by `wc`.

The `wysiwyg` parameter is useful for scaling the image to a full window instead of the same size as the plot. Setting `wysiwyg='n'` sets a full display and `wysiwyg='y'` sets a plot display (the default).

9.6 Integration

This section describes methods and tools for displaying and plotting integrals. Table 39 lists the integration commands and parameters described in this section.

Displaying Integrals Step-by-Step

The following methods should give you an opportunity to compare procedures. Before starting each procedure, be sure to obtain a typical spectrum by entering:
`rt('/vnmr/fidlib/fid1d') wft full`.

Menu Method

1. Click on **Return**.

   The 1D Data Display menu appears. It will also appear after steps 2, 3, and 4.
2. Click on **Massage** > **Region** > **Return**.
3. (Optional) Click on **Massage** > **BC** > **Return**.
4. Click on **Massage** > **Adj IS** > **Return**.
5. Click on **More**.

Table 39. Integral Display and Plotting Commands and Parameters

Commands	
`bc*`	1D baseline correction
`cdc`	Cancel drift correction
`cz<(freq1,freq2,...)>`	Clear integral reset points
`dc`	Calculate spectral drift correction
`dli`	Display list of integrals
`dlni`	Display list of normalized integrals
`dpir`	Display integral amplitudes below spectrum
`dpirn`	Display normalized integral amplitudes below spectrum
`isadj<(size<,neg_size>)>`	Automatic integral scale adjustment
`nli`	Find integral values
`pir`	Plot integral amplitudes below spectrum
`pirn`	Plot normalized integral amplitudes below spectrum
`region*`	Divide spectrum into regions
`z<(reset1,reset2,...)>`	Add integral reset point at cursor position
`* bc<(<1|'unbc',>nsubregion<,minpoints<,minregion>>>)>`	
`region<(tail_length,relative_num,threshold,num_points,`	
`tail_size:<:num_regions>`	
Parameters	
`dcg` {'dc', 'cdc'}	Drift correction group
`ins` {number}	Integral normalization scale
`intmod` {'off', 'partial', 'full'}	Integral display mode
`liamp` {numbers}	Amplitudes of integral reset points
`lifrq` {numbers, in Hz}	Frequencies of integral reset points
`lvl` {number}	Zero-order baseline correction
`tlt` {number}	First-order baseline correction

The 1D Data Display Secondary Menu appears.

6. Click on **Integrals**.

   The text window displays a list of integral intensities.

Fully Automated Method

1. Enter **`intmod='partial' region`**.

   The integral display mode is changed so that only every other integral region is displayed, and the spectrum is automatically broken into integral regions.

2. (Optional) Enter **`bc`**.

   A spline-fit baseline correction is performed to produce the flattest possible baseline.

3. Enter **`isadj`**.

   The largest integral is adjusted to a reasonable size.

4. Enter **`dli`**.

   The text window displays a list of integral intensities.

Manual Method

1. Enter **`cz`**.

   Any currently defined integral reset points are cleared.

2. Enter **intmod='partial'**.

   The integral display mode is changed so that only every other integral region is displayed.

3. Click on **Next** > **resets**.

4. Click the **left button** slightly to the left of the left-most group of peaks.

   This establishes the end of the first (from the left end) section of baseline. You can position the mouse cursor anywhere vertically that seems most comfortable.

5. Click the **left button** slightly to the right of the left-most group of peaks.

   This establishes the end of the first section of peaks.

6. Repeat steps 4 and 5 for each group of peaks across the spectrum. The reset points must alternately separate baseline and peaks. If two peaks are adjacent to each other but you want a reset between them, click the button `twice` at the same place. This establishes a "baseline" region of zero length.

   Note that you can also `add` additional resets in this way to resets that were established automatically by the `region` command.

7. Enter **vp=12**.

   The spectrum moves up to allow space for a numerical display of integrals.

8. Click the **center** mouse button above the right end of any displayed integral.

   This adjusts the integral vertical scale

9. Enter **ins=*x*,** where *x* is the value you wish to assign to the sum of the integrals.

   The value entered affects only printed output, not the trace of the integral.

10. Enter **dpirn**.

    The text window displays a list of integral amplitudes. The sum of the integrals is normalized to the value of the parameter `ins`.

Baseline Correction

Almost all of the operations performed on spectra assume a "good" baseline. Line lists, integrations, resolution measurements, 2D volume integrations, etc., all measure intensities from "zero" and do not perform any baseline adjustments. If the baseline in your spectrum is not "good," you should first perform a baseline correction operation before performing further data reduction. Two types of baseline correction are provided: linear and non-linear.

The `dc` command turns on a linear baseline correction, using the beginning and end of the displayed spectrum to define a straight line to be used for baseline correction. The result is to calculate a zero-order baseline correction parameter `lvl` and a first-order baseline correction parameter `tlt`. The `cdc` command turns off this correction. The results of the `dc` or `cdc` command is stored in the `dcg` parameter, which can be queried (`dcg?`) to determine whether drift correction is active. If active, `dcg=''`; if inactive, `dcg='cdc'`.

The `bc` command turns on 1D and 2D baseline correction. The 1D baseline correction uses spline or second to twentieth order polynomial fitting of predefined baseline regions. `bc` defines every other integral, that is, those integrals that disappear when `intmod='partial'` as baseline and attempts to correct these points to zero. A variety of parameters can be used to control the effect of the `bc` command.

For more information about the `bc` command, refer to the entry for `bc` in the *VNMR Command and Parameter Reference*.

Integral Reset Points

The `z` command (or the equivalent function key) resets the integral to zero at the point marked by the displayed cursor. `z(reset1,reset2,...)` allows the input of the reset points as part of the command, instead of using the position of the cursor. Reset points do not have to be entered in order. The resets are stored as frequencies and will not change if the parameter `fn` is changed. The command `cz` removes all such integral resets. `cz(reset1,reset2,...)` clears specific integral resets.

For a list of integrals, the `liamp` parameter stores the integral amplitudes at the integral resets points and the `lifrq` parameter stores the frequencies of integral reset points. To display the values of `liamp`, enter `display('liamp')`. Frequencies are stored in Hz and are not adjusted by the reference parameters `rfl` and `rfp`.

Integral Regions

The `region` command divides a spectrum up into regions containing peaks. A variety of parameters can be used to control the effect of the `region` command; see the *VNMR Command and Parameter Reference* for details.

Integral Display and Plotting

Display and plotting of the integral trace is independent of the values of the integrals. The height of the trace is controlled by the parameter `is` and can be interactively adjusted with the `ds` command. Also, the macro `isadj(height)` adjusts the integral height so that largest integral fits the paper or is `height` mm tall if an argument is provided, for example, `isadj(100)`.

The command `dli` displays a list of integral values at the integral reset points. The frequency units of the reset points are defined by the parameter `axis`. The reset points are stored as Hz and are not referenced to `rfl` and `rfp`. The amplitudes are stored as actual values; they are not scaled. The integral values are scaled by the parameters `ins` and `insref` and the Fourier number. Typically, `ins` is set to the number of nuclei in a given region. For example, if a region represented a single methyl group, the following procedure would scale the integral values of that region:

1. Set **`ins`**=**3**.
2. Set **`insref`** to the Fourier-number-scaled-values of that integral.
3. Enter **`dli`**. The integral value of that region is displayed as 3 and all other integral values are accordingly scaled.

Integral value scaling can be interactively set with the `ds` command. The `setint` macro can also be used to adjust integral value scaling. `setint` sets the value of an integral and is used in conjunction with the command `dli` to scale integral values.Normalized integral values can also be selected. In this case, `ins` represents the total number of nuclei. The individual integral values will be scaled so that their sum is equal to `ins`. The normalized mode may be selected by setting `insref` to “not used.” The integral is scaled by `ins` and `insref`.

Two commands are closely related to `dli`:

- `nli` is equivalent to `dli` except that no screen display is produced.
- `dlni` normalizes the values from `dli` using the integral normalization scale parameter `ins` and then displays the list.

The `dpir` command displays numerical integral values below the appropriate spectral regions, using the integral blanking mode in which only every other integral is plotted. The command `dpirn` shows the normalized integral values in an analogous fashion.

The `pir` command plots digital integral values below the spectrum, using the integral blanking mode in which only every other integral is plotted. The command `pirn` plots the normalized integral values in an analogous fashion.

9.7 Plotting

VNMR software allows plotting in a multiprocessing, multiuser environment. A plotter can be shared between several users and/or processes that generate plots at the same time. A plotter can even be shared between multiple VNMR instruments and workstations, as long as they are connected to each other via Ethernet. On the other hand, one system can support multiple plotters, which permits use of the optimal device for each task. Table 40 lists commands and parameters associated with plotting.

Table 40. Plotting Commands and Parameters

Commands	
`ap<(template)>`	Print out all parameters
`bpa:$sc2_minimum`	Plot boxed parameters
`hpa`	Plot parameters on special preprinted chart paper
`killplot`	Stop plot job and remove from plot queue
`page<(num_pages<,'clear'|file>)>`	Submit plot and change plotter page
`pap<(<template,>x,<,y><size>)>`	Plot out “all” parameters
`pltext*`	Plot text file
`ppa<(x<,y>)>`	Plot parameter list in “English”
`setpen<(maxpen,max_num_pen)>`	Set maximum number of HP pens
`setplotdev<:plotter_type>`	Return characteristics of a named plotter
`showplotq`	Display plot jobs in plot queue
`showplotter`	Display currently defined plotters and printers
`vnmrplot <file>`	Plot files (UNIX)
`* pltext<(<file><,x<,y<,width>>>)> <:$x_next,$y_next,$y_increment>`	
Parameters	
`ap` {string}	“All” parameters display control
`maxpen` {1 to number of pens}	Maximum number of pens to use
`plotter` {string}	Plotter device
`wcmax` {number, in mm}	Maximum width of chart
`wc2max` {number, in mm}	Maximum width of chart in second direction
`x0` {number, in mm}	X-zero position of HP plotter or Postscript device
`y0` {number, in mm}	Y-zero position of HP plotter or Postscript device

Plotter Output

Plotting in a multiuser environment is controlled by “pages.” Each plot produces a one “page” output on the selected plotter device (note that on certain plotters, such as the Zeta plotter, one “page” might be physically several fanfold pages long). Multiple commands, which may in fact be separated by a long delay, can produce one page.

A page is started by any one of the legal plotter commands. It can be followed by any other plotter commands. All these commands immediately calculate the appropriate plotter information, which is then stored in an intermediate file (or memory buffer in the case of

raster graphics printers). Finally, each plot or group of plots is terminated by the page command. page closes the current page and submits it to the appropriate plotter queue, where it is sent to the plotter as soon as possible. page also requests a new page on those plotters equipped with an automatic paper changer.

The UNIX command vnmrplot is installed as part of the VNMR system to plot files from inside VNMR commands. The showplotq macro displays the current plot jobs in the plot queue for the active plotter.

To stop a plot in progress (a plot in which you have not entered page), use the command page('clear'). The killplot macro stops all current plot jobs in the plot queue for the active plotter, then removes the jobs from the plot queue. Unless the user executing killplot is root, only that user's plots jobs are deleted from the plot queue.

Plots can be sent to a file instead of to a plotter by supplying a file name argument to the page command. In this way, PCL, HP-GL, and PostScript files can be captured for incorporation into other computer documents.

Plotter Configuration

The VNMR software supports a variety of different plotter devices with different characteristics. Pen plotters and raster graphics printers are supported. For pen plotters, the HPGL graphics language from Hewlett-Packard is used. For raster graphics printers, the Hewlett-Packard raster mode or PostScript is used. The following parameters are used to describe the characteristics of different plotters:

- plotter contains a code for the selected plotter.
- wcmax is the maximum horizontal width, in mm, of the plotter area.
- wc2max is the maximum vertical size, in mm, of the plotter area.
- maxpen is the maximum number of pens (colors) available on plotter. When changing to a Hewlett-Packard plotter, the setpen macro allows the user to interactively define the maximum number of pens.

The parameters plotter, wcmax, wc2max and maxpen are global and have an effect on all experiments (exp1 through exp9) simultaneously. wcmax, wc2max and maxpen are set up during the plotter configuration to certain values but can be changed by the user. Certain maximum plotter values, as listed below, cannot be exceeded. The following Hewlett-Packard pen plotters are supported:

Plotter Type	*Paper Size*	*Code*
DraftMaster	ABCDE	DraftMaster_A, etc.
DraftPro	C, D	DraftPro_C, DraftPro_D
HP 7475A	B	HP7475A
HP 7550A	A, B	HP7550A8, HP7550A

The following Hewlett-Packard and Postscript raster printers, which can effectively act as plotters, are supported:

Printer Type	*Paper Size*	*Dots/inch*	*Code*
LaserJet Plus	11 × 8	150, 300	LaserJet_150, LaserJet_300
QuietJet Plus	14 × 11	96, 192	QuietJet_96, QuietJet_192
ThinkJet	8 × 11	96, 192	ThinkJet_96, ThinkJet_192

Printer Type	*Paper Size*	*Dots/inch*	*Code*
Postscript	8 × 11		PS_A
Postscript	11 × 8		PS_AR

Default configuration and maximum values for plotters and printers are the following:

Plotter	*Configuration Values*			*Maximum Plotter Values*		
Code	wcmax	wc2max	maxpen	wcmax	wc2max	maxpen
HP7475A	400	210	6	400	210	6
HP7550A8	250	155	8	250	155	8
HP7550A	400	210	8	400	210	8
DeskJet_300	200	140	1	200	140	1
DeskJet_30R	240	180	1	240	180	1
DraftPro_C	520	350	8	520	350	8
DraftPro_D	800	480	8	800	480	8
DraftMaster_A	220	140	8	220	140	8
DraftMaster_B	370	225	8	370	225	8
DraftMaster_C	520	350	8	520	350	8
DraftMaster_D	800	480	8	800	480	8
DraftMaster_E	1000	780	8	1000	780	8
ThinkJet_192	200	115	1	200	240	1
ThinkJet_96	200	115	1	200	240	1
QuietJet_192	330	230	1	330	240	1
QuietJet_96	330	230	1	330	240	1
LaserJet_150	200	105	1	200	150	1
LaserJet_150R	200	105	1	250	180	1
LaserJet_300 (a)	200	105	1	200	240	1
LaserJet_300R (a)	200	105	1	250	180	1
LJ_B300R	400	210	1	400	210	1
LJ_A3_300R	380	235	1	380	235	1
LaserJet_600	200	105	1	200	140	1
LaserJet_600R	200	105	1	250	180	1
PS4079_HPGL	400	205	1	400	205	1
PS_A	180	140	1	180	140	1
PS_AR	250	155	1	250	155	1

(a) The standard LaserJet Plus in its high-resolution mode (plotter code `LaserJet_300`) can only support `wcmax*wc2max<=200*105`. If `wc2max` is increased above 105, `wcmax` has to be reduced accordingly. This restriction does not apply if the 2-Mbyte memory expansion has been installed in the LaserJet Plus.

Plotter Resolution and Speed

Pen plotters operate at a fixed resolution. For raster graphics printers (ThinkJet, LaserJet, etc.), a high-resolution and a medium-resolution mode is provided:

- The high-resolution mode (the plotter code with the larger number appended, e.g., LaserJet_300) should be used for high-quality 1D NMR spectra and grayscale images.
- The medium-resolution mode (e.g., `LaserJet_150`) should be acceptable for 2D contour maps.

The times required to plot a complete drawing on pen plotters depends on the number and size of the individual vectors in the drawing. On raster graphics printers, the time required to complete a drawing depends on the size of the drawing (`wcmax` and `wc2max`) and on the resolution. The high-resolution mode is usually about four times slower than the medium-resolution mode. The ThinkJet and the LaserJet use 8.5 × 11 in. paper.

Selecting a Plotter

From the Main Menu, select the More button, followed by Configure, then Show Output Devices, which invokes the showplotter macro to list the current plotter as well as your possible choices. Select Plotter will step through the various choices.

Alternatively, type in the name of the plotter, such as `plotter='HP7550A'`. This will run the `setplotdev` macro to configure the system for this plotter. During the configuration, `wcmax`, `wc2max` and `maxpen` are set to the values described in table above but can now be changed to smaller, and in some cases larger values, if required. After the system has been configured for a given plotter, the graphics display window represents the plotter graphics area.

Never change the plotter configuration during the preparation of a single output page, because all commands of one page will go to the same plotter. If several plotters are connected to the system, it is possible to change the plotter definition between pages, even if these pages are still waiting in a queue to be printed.

The plotter configuration is stored in global variables for each user. Therefore, each user can have their own plotter definition, but all foreground and background tasks for one user will share the same information. There is one exception to this rule. If a plotter configuration command is placed within a macro command, which is executed in background, it will only be valid during and within the execution of that background task. This is in fact true for any one of the “global” parameters.

Color Printing

The `color` program allows you to change the colors on the VNMR display screen and color print to raster plotters and pen plotters.

Starting the Color Program

To start the program, enter `color` on the VNMR command line.

A color selection window, shown in Figure 68, opens.

The default window is for General (or 1D phase) color selection for the graphics window (Display). To change to other color selection windows, click on the buttons near the top of the VNMR Color Selection window to display the 2D Phase, 2D Absolute Value, and Image color selection windows:

- The General window has buttons along the left side that list the areas of the graphics window for which you can set colors: background, spectrum, integral, fid, imaginary, scale, parameter, cursor, and threshold. To the right of each button is the color currently assigned for that area of the graphics window.

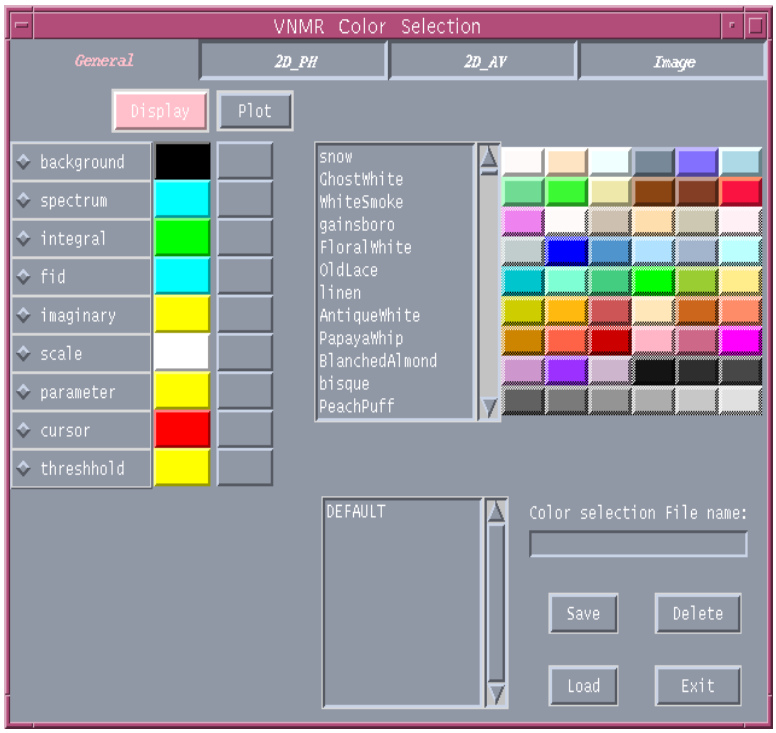


Figure 68. Color Selection Window (`color` Program)

- The buttons for the 2D Phase window for the display, shown in Figure 69, allow you to set colors for the contours of the display.
- The buttons in the 2D Absolute Value window for the display, shown in Figure 70, allow you to assign colors to the contours of the display.
- The Image window for the display, shown in Figure 71, allows you to set the colors for the display background and foreground.

Setting Colors

You can select colors from either the color list box (in the center of the window) or the color palette. For every color on the palette, there are ten values in the list box. To set the background color of the graphics window to gray, for example, do the following steps:

1. Click on the background button.
2. Click on a gray button in the color palette.

   The name of the button and its values appear in the scrollable list box directly to the left of the palette. To change the color shade, click on a value in the list (e.g., gray13).

To set colors for the remaining eight areas of the display, repeat steps 1 and 2.

Saving A Color File

When you are satisfied with the color assignments, you can save them in a file as follows:

1. Enter a name in the Color Selection File Name field in the bottom right-hand corner of the Color Selection window. The bottom list box is updated with the new file name.

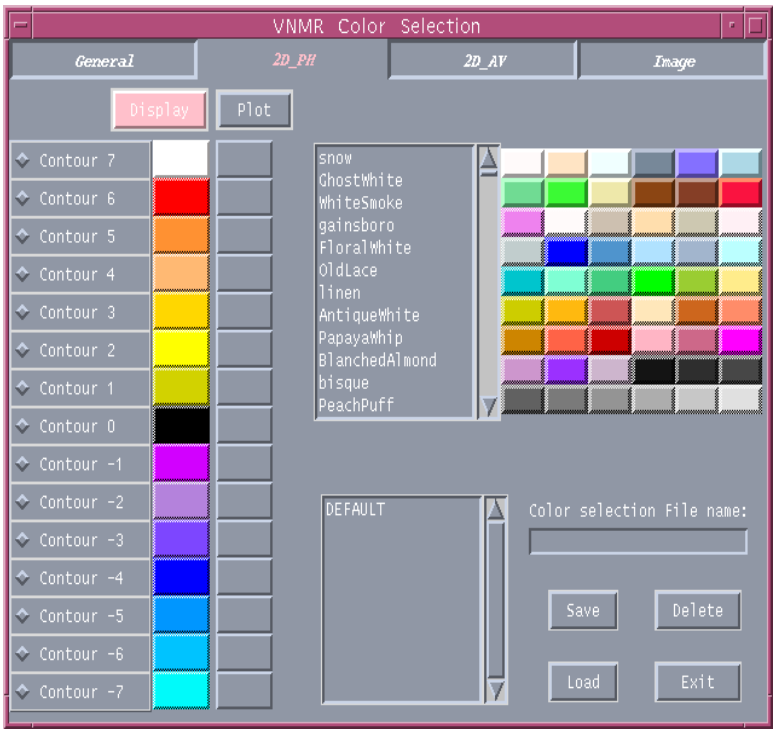


Figure 69. 2D Phase Color Selection Window (`color` Program)

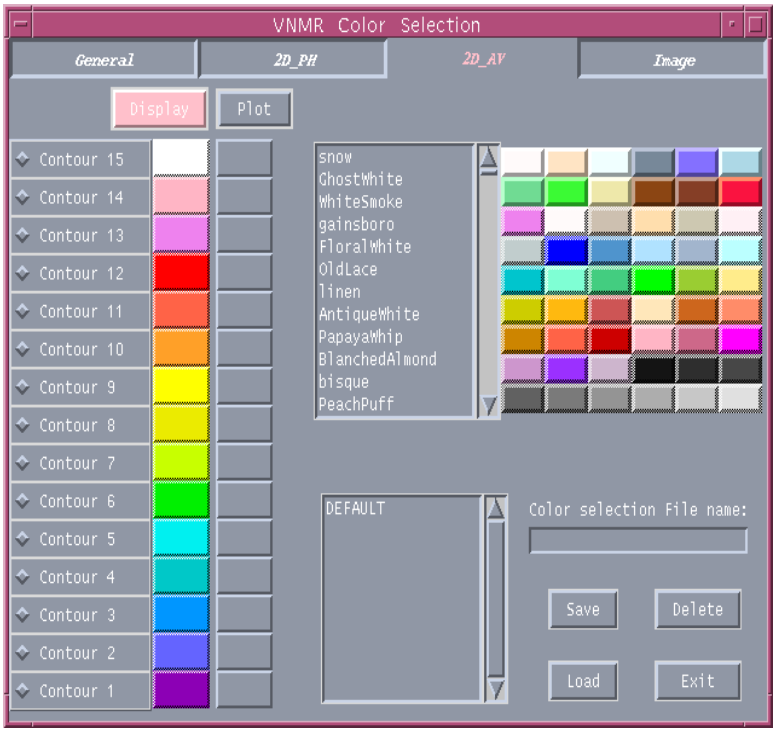


Figure 70. 2D Absolute Value Selection Window

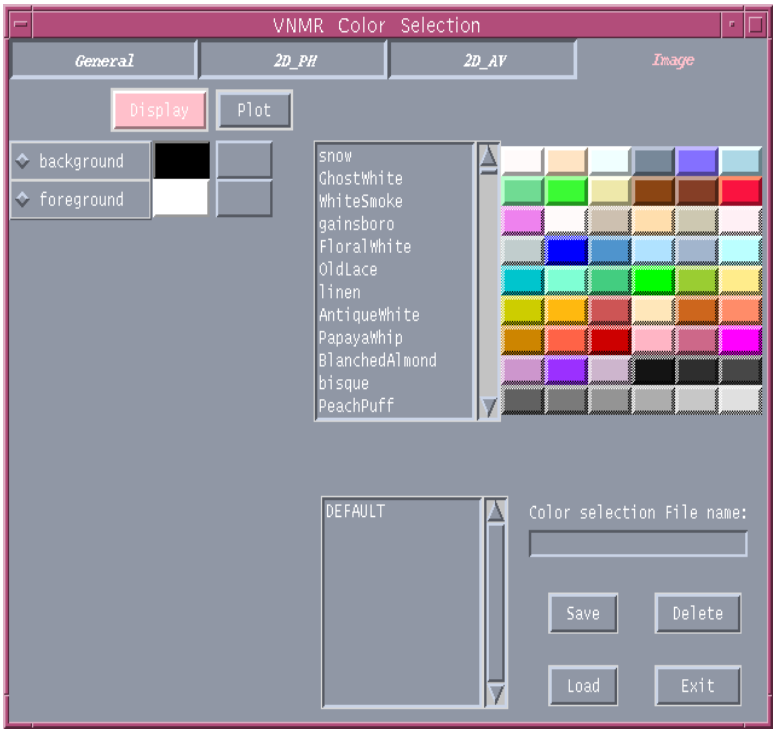


Figure 71. Image Color Selection Window

2. Click on the Save button. The color file is saved in the designated place in the VNMR system file.

Loading A Color File

To retrieve a color file:

1. Click on the color file name in the scrollable list box at the bottom of the window. The color file name appears on the entry area of the Color Selection File Name field.
2. Click on the Load button.

Changing or Renaming A Color File

To change the colors in a file:

1. Load the file.
2. Enter new color assignments.
3. Save the file.

To change the name of a color file:

1. Load the file.
2. Save the file with a new name.
3. Delete the file with the old name.

Removing A Color File

To remove a color file from the list:

1. Click on the file name.
2. Click on the Delete button. The deleted file is removed from the bottom list box.
3. When you are prompted, choose OK to delete the file, or Cancel to keep the file.

Assigning Colors to A Plotter

To assign colors to a plotter:

1. Click on the Plot button.
2. Choose the type of plotter that you have.

   Use the previously listed procedures to save, load, change, rename, and remove files.

To use normal plotting commands:

1. Exit the Color Selection window.
2. Enter `setcolor` on a command line.

Closing the Color Selection Window

When you have finished using the program, click on Exit to close the window.

Color Table Loader

The macro `loadcolors<(color_file)>` loads the color table for the graphics window and plotters. `loadcolors` is generated by the `colors` program and includes a series of `setcolor` commands. On bootup, the `bootup` macro calls `loadcolors` to set the graphics window and plotter colors.

Plotting Parameter Lists and Text Files

A number of commands and macros are available for plotting lists and text files:

- `ppa<(x<,y>)>` prints the most important parameters in an “English-language” format, with full explanation of each parameter. If the `x` and `y` coordinates are given as arguments, the plot can be positioned as desired. The coordinates control the x and y offset, in mm, from the lower left of the plot to the starting position at the upper left.
- `bpa` plots a box around the entire chart (assuming blank paper) and then plots “chemist-style” parameters in boxes along the lower edge of the chart. `bpa` is the same as `ppa`, but with a different layout. Both `ppa` and `bpa` behave somewhat naively if the pulse sequence is more complex, but they were designed primarily for chemists, not for spectroscopists.
- `pap<(<template,>x,y<,character_size>)>` also plots parameters but it uses a “mnemonic” format, listing only the two- or three-character names and values of all the parameters. The `ap` parameter controls display of `pap`. Use the command `paramedit('ap')` to modify the string value of `ap`. See the *VNMR User Programming Manual* for information on the `template` argument. The `x` and `y` arguments are the same as `ppa` above. For `pap` only, a character size can be specified as a multiplier—the default is 0.7.
- `ap<(template)>` prints out all parameters in the parameter list. The `ap` parameter controls display of the `ap` command. Use `paramedit('ap')` to modify the string

value of ap. See the manual *VNMR User Programming* for information on the template argument.

- hpa "fills in the blanks" on the bottom of the preprinted chart paper available for Hewlett-Packard 7475A and 7550A plotters. The x0 and y0 parameters adjust the x-zero and y-zero positions in mm, respectively, of Hewlett-Packard plotters and Postscript devices. You can use hpa to adjust x0 and y0 so that the numbers that are filled in on the blank lines are in a pleasing position.
- pltext<(<file><,x<,y<,width>>>)> <:$xn,$yn,$y_inc> plots the text contents of a file on the plotter. The default is the current experiment text file. x and y are the coordinates, in mm, of the first line of text. width is the maximum column text width, in characters. pltext uses a word wrap to make the text fit into the width specified.

9.8 Plot Designer

Plot Designer allows you to see and design a plot before you print it. It provides templates, drawing tools, and a text editor that give you the capability of positioning spectra, parameters, axes, and other plot output on a page.

System Requirement

Plot Designer is a Java-based application.You must have Solaris 2.6 or later installed in order to use Plot Designer. The Java™ Runtime Environment (JRE) for Solaris™ from Sun Microsystems provides an environment in which you can run Java applications. You can download the latest version of JRE for Solaris™ from the Sun Microsystems Web site at http://www.sun.com/solaris/jre/index.html.

Starting Plot Designer

Start the Plot Designer program by entering the macro jdesign or the command jplot('-setup') in the VNMR input window.

This opens the Plot Designer window, shown in Figure 72.

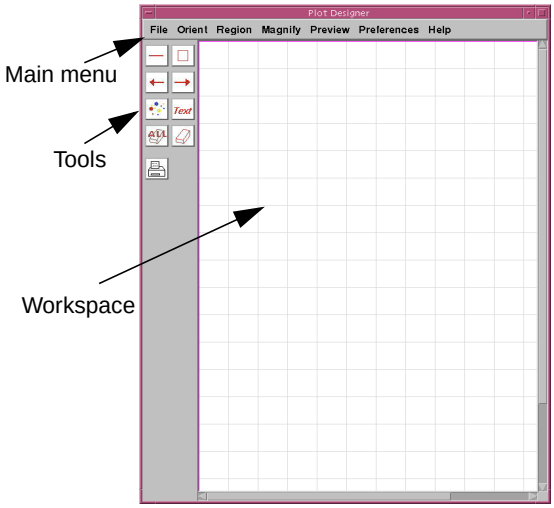


Figure 72. Plot Designer Window

Customizing the Plot Designer Window

You can easily change the size and appearance of the Plot Designer window by doing the following procedure:

1. Click on **Preferences** in the main menu, then **Set Up** to open the Window Preferences panel shown in Figure 73.
2. To change an aspect of, or property in, the Plot Designer window, click on its corresponding button to open a pull-down menu.

   See Table 41for a description of each control.

   Figure 74 is an example of the window without visible region borders and without a grid.

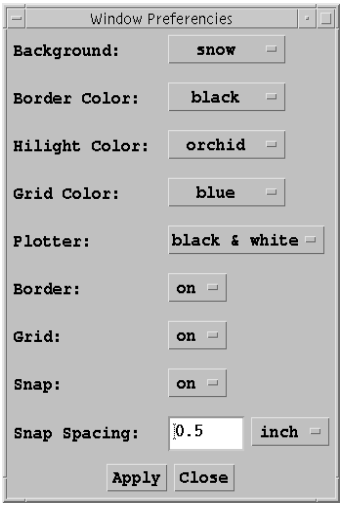


Figure 73. Window Preferences Panel

Table 41. Window Preference Controls

Control	*Function*
Background	Changes the background color of the window.
Border Color	Changes the color of the border surrounding the workspace.
Highlight Color	When you double-click on an object, its color changes to indicate that it is highlighted. This option controls the highlight color.
Grid Color	Changes the color of the grid.
Plotter	Allows you to choose a black and white or color plotter.
Border	Shows (**on**) and hides (**off**) region borders.
Grid	Shows (**on**) and hides (**off**) grid in the workspace.
Snap	The grid has magnetic properties. When snap is turned **on**, the path of an object (the center of its border) automatically snaps to the grid whenever you draw or move the object or change its size or shape. Turning **off** Snap demagnetizes the grid.
Snap Spacing	Controls the amount of space on the grid to which an object snaps. Spacing can be in inches, centimeters, or points.

3. After you have entered all of your preferences, click **Apply** to execute the changes.
4. Click **Close** to exit the window.

Customizing a Plot

You can add simple graphics and text to a plot and change its size and appearance by using the tools listed in Table 42. To use a drawing tool, press and hold down the left mouse button and drag the cursor in the workspace.

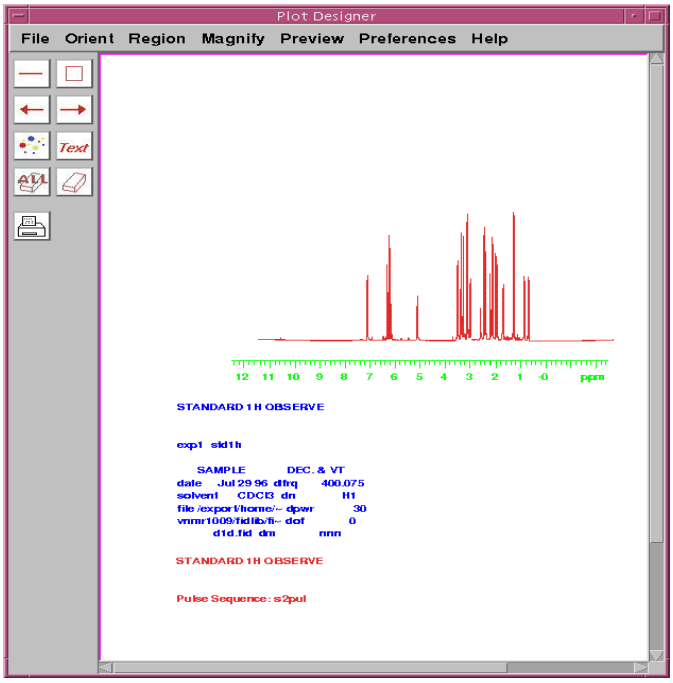

Plot Designer
File Orient Region Magnify Preview Preferences Help
Text
12 11 10 9 8 7 6 5 4 3 2 1 0 ppm
STANDARD 1H OBSERVE
exp1 sid1h
SAMPLE DEC. & VT
date Jul 29 96 dfrq 400.075
solvent CDCl3 dn H1
file /export/home/~ dpwr 30
vnmr1009/fidlib/fi~ dof 0
d1d.fid dm nnn
STANDARD 1H OBSERVE
Pulse Sequence: s2pul

Figure 74. Window with Data and Without Borders and a Grid

Using Templates

You can create your own templates. After you have created a design, do the following procedure to save your design as a template:

1. Click **File**-**Templates** to open the Plot Templates window.
2. Enter a name in the **Template** field. If you want the file to be the default template, click the box next to **Use this template as default**. After you select a file as a template, the next time that you start Plot Designer, it will automatically open with the template.
3. Click **Save** to store the template in `$vnmruser/template/plot` directory.

   If you try to save a template with the same name as an already existing template, a warning notifying you that the file will be overwritten appears. If you do not want the file replaced, click **Cancel**.
4. Quit the Plot Templates window by clicking on **Close**.

Loading a Template

After you have created templates, you can run Plot Designer with a specific template by typing the `jplot` command and the template name. For example, entering `jplot('t1')` starts Plot Designer with the t1 template automatically loaded.

If you opened Plot Designer with the `jdesign` macro, the workspace will either be empty or contain the design that was being worked on the previous time Plot Designer was used. Do the following procedure to load a template file:

1. Click on **File** in the main menu, then **Templates** to open the Plot Templates window.
2. Highlight (select) a template by either DOUBLE-CLICKING on a file in the list in the upper region of the window or by entering the file name in the **Template** field.

Table 42. Plot Designer Tools

	Line Drawing	Draws a line.
	Box	Draws a box.
	Arrows	Draws an arrow; places the arrowhead at the point in which you START to draw the arrow.
		Draws an arrow; places the arrowhead at the point in which you END drawing the arrow.
	Item Preferences	Sets the color and size of lines and fonts. To edit an object, highlight it by double-clicking on it. For a description of its properties, see page 267. You can also open this tool by clicking on **Region-Preferences**.
	Text Input	Allows you to add text into your design. Several options allow you to control the size and appearance of the text. To use this tool, see “Adding Text” on page 269
	Erasers	The **ALL** eraser removes all objects. You can also remove selected objects by using the **Region-Delete All** option described on page 267.
		The second eraser removes only selected objects. You can also remove selected objects by using the **Region-Delete** option described on page 267.
	Print	Prints a file.

If you want the file to be the default template, click on the field **Use this template as default**.

3. To insert the template into the Plot Designer window, click on **Open**.
4. Click **Close** to exit the window.

Removing Templates

To remove a template from the list in the Plot Templates window, click on **Delete**. A warning appears notifying you that the template will be deleted. Click **Cancel** if you do not want to delete the template.

Importing a Plot

To import a plot from the VNMR graphics window onto the Plot Designer workspace, you must first create a region. Regions are smaller workspaces in which you can customize a plot. Create a region by doing the following procedure:

1. Click on **Region** in the main menu, then **New** to create a region on the workspace. The cursor arrow changes to cross-hairs.
2. To draw a region, press and hold down the left mouse button, drag the cursor across the workspace, then release the mouse button.
3. If a region is not already selected, highlight it, then click **Region-Edit** to open the Region Editor window shown in Figure 75. Region Editor is a text editor in which you can enter commands to change an imported plot.

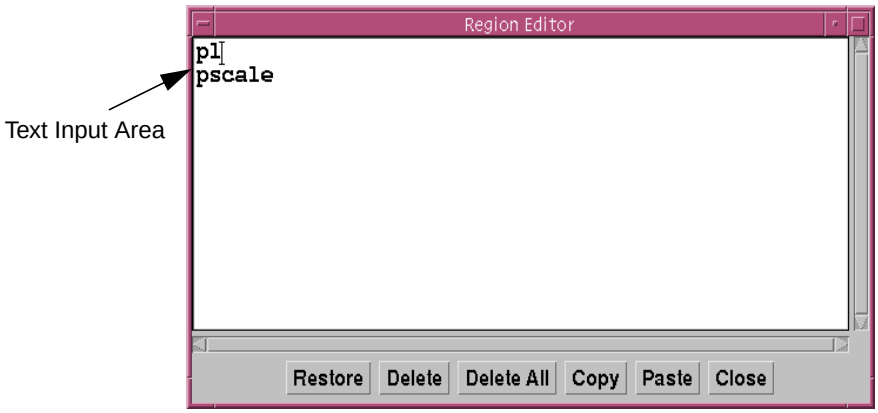


Figure 75. Region Editor Window

4. Enter a VNMR command (such as `pl` or `pscale`) in the text input area.
5. Click **Preview-Selected** to import the plot into the region. Click **Preview-All** to import plots into multiple regions.

You can also import a plot into a region by doing the following procedure:

1. Click on **Region-Edit** to open the Region Editor.
2. Draw a region.
3. Press the right mouse button to open the plot menu window

.
4. Choose a command to import into the Region Editor.

Commands are stored in the `/$vnmruser/templates/plot/menu` file or `/$vnmrsystem/user_templates/plot/menu` file. You can edit both of these files to add or delete commands. In the `menu` file, the command is indicated by two lines: the first line is the label of the command that appears in the plot menu window; the second line is the command itself. In Figure 76, the label `pl` identifies the command line `pl pscale`. The label `PAP` identifies the `pap` command.

Editing a Plot

To edit a plot, do the following procedure:

1. Highlight a region.
2. Click **Region-Edit** to open the Region Editor window.
3. Enter a command (such as `p1` or `pscale`) in the text input area. Use the buttons listed in Table 43 to edit text.
4. Exit Region Editor by clicking **Close**.

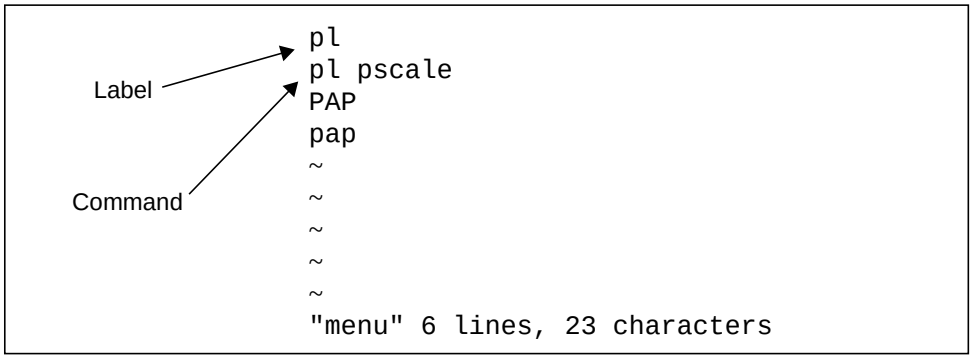


Figure 76. `menu` File

Table 43. Region Editor Buttons

Button	*Function*
Restore	Applies the original template to a region. If you opened a template and made changes to it, you can restore it to its original design by using this button.
Delete	Removes text. This option is not similar to **Copy**. Deleted text is not stored in a buffer; do not use **Delete** to cut and paste text.
Delete all	Clears all text from the input area.
Copy	Duplicates text.
Paste	Inserts copied text in the input area.

Deleting a Region

To delete a region from the workspace, highlight the region, then click **Region-Delete**. Click **Region-Delete All** to remove all regions.

Note: Regions removed with **Delete All** are not stored in a buffer and cannot be restored to the workspace.

Restoring a Deleted Region

To restore a *single* region deleted from the workspace, click **Region-Undelete**. Regions removed with **Delete All** cannot be restored with **Undelete**.

Clearing the Workspace

To *permanently* remove all regions from the workspace, click **Delete All**. Remember, if you remove all regions, you cannot restore them with **Undelete**.

Customizing Objects in a Region

You can change the size and color of objects in a region with the Item Preferences window shown in Figure 77. Click on **Region-Preferences** to open this window. You can also open the window by clicking on the Item Preferences tool , described on page 265.

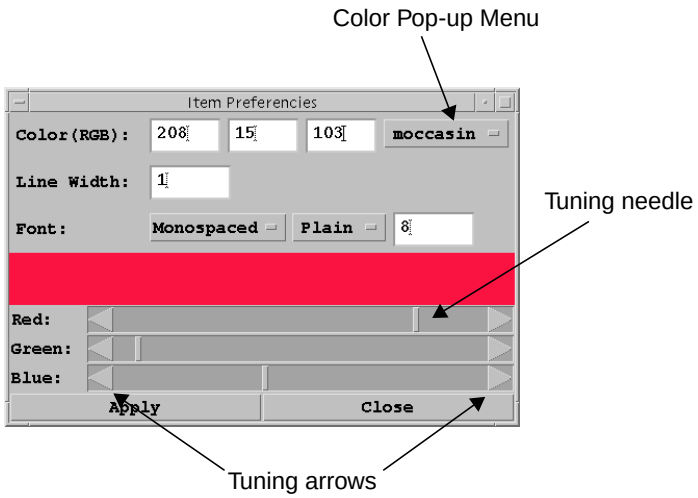


Figure 77. Item Preferences Window

Changing Line Width

Change the width of a line by doing the following procedure:

1. Highlight the line or region by double-clicking on it.
2. Enter a new width in the **Line Width** field.
3. Click **Apply** to change the line.
4. Click anywhere in the workspace to deselect the line.

Changing Fonts

Plot Designer has three font families: SansSerif, Monospaced, and Serif. Fonts can be Plain, **Bold**, or *Italic*. To change the family, style, and size of a font, do the following procedure:

1. Highlight the text or region.
2. Click on the Item Preferences tool to open the Item Preferences window.
3. Choose a family, style, and enter a size in the **Font** field.
4. Click **Apply** to change the text.

Changing Line Color

You can change the color of a line by doing the following procedure:

1. Highlight the line or region.
2. In the Item Preferences window, click on the color button

to open a pop-up menu showing a range of colors.
3. Move either the tuning needle left or right to change a color. You can also change a color by clicking on the left or right arrows in the **Red**, **Green**, and **Blue** fields; the values in the **Color(RGB)** field automatically change as you move a needle.
4. When you are satisfied with a color, click **Apply**.
5. Place the cursor anywhere in the workspace and click once to see the color change.

Adding Text

To add text into your design, do the following procedure:

1. Click on the text input tool Text to open the text input window.
2. Type text in the field at the top of the window.

   You can customize your text by clicking on the desired options and entering a font size in the indicated field.
3. Click on **Put** and drag the cursor into the workspace, then click once to paste in the text.

To copy text that is already on the workspace and paste it in different font styles, do the following procedure:

1. Highlight the text.
2. Open the Text Input window shown in Figure 78 by clicking the text input tool Text .

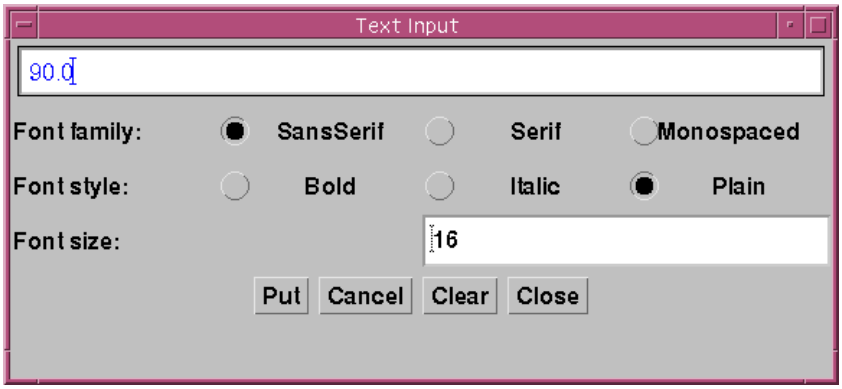


Figure 78. Text Input Window

3. Select a **Font family** and **Font style**, and enter a **Font size**.
4. Click **Put** to paste the text in the workspace.

Changing Font Color

To change the color of fonts, repeat the procedure for Changing Line Color.

Adjusting and Restoring Plot Parameters

When you draw a region, the scaling parameters of the plotting area (`wcmax` and `wcmax2`) are adjusted by the macro `jplotscale`. The scaling parameters of a plot that is imported into a region (`io`, `is`, `vs`, `wc`, and `wc2`) are automatically adjusted according to `wcmax` and `wcmax2`. If you want to use the adjusted parameters, enter the following command string, which first restores the parameters of the current experiment (`n`) to the plot, then applies the adjusted parameters to the plot:

```
jplotunscale jexpn jplotscale
```

If you do not want to use the adjusted parameters, enter the following command:

```
jplotunscale jexpn
```

`jplotunscale` is a macro that restores the original parameters of the current experiment to the plot.

Moving Objects and Changing Object Size

You can move an object by double-clicking on it and dragging the mouse across the workspace. To move a region, click anywhere inside the region or on its border.

You can shrink or enlarge an object by double-clicking on it, placing the cursor on a border anchor and dragging it.

Changing the Shape of the Plot Designer Window

Plot Designer can be viewed in two orientations, **Landscape** or **Portrait** (which is the default orientation). You can change the shape of the Plot Designer window in the **Orient** menu.

Changing the Size of the Plot Designer Window

Increase or decrease the size of the Plot Designer window by clicking on the sizes listed in the **Magnify** menu.

Saving Your Plot

After you are satisfied with the plot that you have created, do the following procedure to store your file:

1. Click on **File** in the Main Menu, then **Save Data** to open the Plot Save window shown in Figure 79.
2. Scroll down the list of directories and choose a directory. You can also enter a path for your file in the **Directory** field.
3. Select a **Data format** for your file and enter a **Data resolution**.
4. Label your file by entering a name in the **File** field.
5. Click **Close** to exit the window.

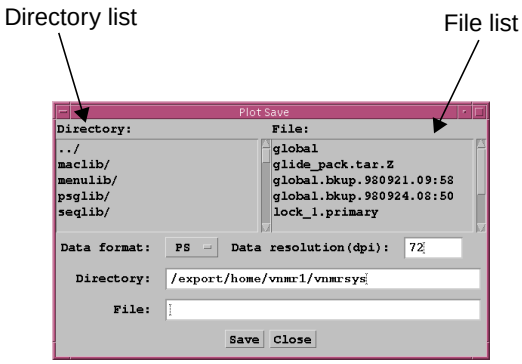


Figure 79. Plot Save Window

Printing Your Plot

To print your plot, click on the print tool .

Getting Help

Click on the **Help** option for descriptions of Plot Designer features.

Exiting Plot Designer

To exit the program, click on **File-Quit**. If you leave a design in the window when you exit Plot Designer, your design will automatically appear in the workspace the next time that you use the program.

9.9 Printing

Table 44 lists printer-associated commands and parameters.

Table 44. Printer-Associated Commands and Parameters

Commands	
`killprint`	Stop print job and remove from print queue
`printoff<('clear'|file)>`	Stop sending text to printer & start print operation
`printon`	Direct text output to printer
`ptext(file)`	Print out a text file
`showplotter`	Display currently defined plotters and printers
`showprintq`	Display print jobs in print queue
`vnmrprint*`	Print text files (UNIX)
`* vnmrprint printfile <printcap> <printer_type <clear|file>>`	
Parameter	
`printer` {string}	Printer device

Printing from within VNMR is initiated with the `printon` command. All output which normally appears in the text window is saved and, when the `printoff` command is issued, sent to a printer. This output includes the following:

- Parameter listings from `dg`, `dg1`, `da`, etc.
- Line listings from `dll`.
- Integral listings from `dli`.
- System configuration parameters generated by `config('display').`
- Text files using the `text` command
- Results of calculations from `h2cal`, `adept`, `t1`, `t2`, etc.
- Any other information that some program or macro may write to the text window.

This output is saved in a temporary file in the VNMR subdirectory `tmp`. The VNMR parameter `printer` determines the printer to which the output is directed. To select a printer, select the More button from the Main Menu, followed by Configure, then Show Output Devices, which invokes the `showplotter` macro to list the current printer as well as your possible choices. Select Printer will step through the various choices. For more information, refer to “Plotting” on page 254.

When the `printoff` command is issued, VNMR executes a UNIX script called `vnmrprint` that sends the temporary file to the printer using standard UNIX printing utilities. This script is supplied with the name of the temporary file to be printed, the name of the printer (corresponding to a `printcap` entry), and the type of printer (corresponding to a `devicetable` entry). (Note that `devicetable` information is used to distinguish PostScript printers.) If desired, the script `vnmrprint` affords a place for user customizing.

The macro `ptext(file)` prints out the text file given as an argument. For example, the command `ptext('/vnmr/psglib/dept.c')` prints the text file `dept.c`.

Print jobs for the currently active printer in VNMR are held in a print queue. The `showprintq` macro displays the current print jobs in the print queue. The `killprint` macro will stop a print job and remove it from the print queue. Unless the user executing this macro is `root` (superuser), only that user's print job is deleted from the print queue.

9.10 User-Controllable Line Drawing

The `pen`, `move`, and `draw` commands provide the user with a line-drawing capability for display on the graphics screen or output on the plotter. By default, the output device is the plotter (`'plotter'`) but the device can be changed to the graphics screen (`'graphics'`) in any of these commands. The output currently selected is passed to subsequent `pen`, `move`, and `draw` commands and remains active until a different output is specified. The commands are entered as follows:

- `pen(<'graphics'|'plotter',><'xor'|'normal',>pen|color)` selects the pen for a plotter (`'pen1'`, `'pen2'`, etc.) or the active color for the graphics screen (`'red'`, `'green'`, `'blue'`, `'cyan'`, `'magenta'`, `'yellow'`, `'black'`, or `'white'`), for example, `pen('graphics','red')`. A drawing mode (`'xor'` or `'normal'`) for the graphics window output can be specified. In the `'xor'` mode, if a line is drawn such that one or more points of the line are in common with a previously drawn line, the common points are erased. In the `'normal'` mode, the common points remain. The default mode is `'normal'`.
- `move(<'graphics'|'plotter'>,x,y)` sets an absolute location with coordinates *x* and *y*, such as `move(10,20)`. This becomes the point from which to start drawing the line.
- `draw(<'graphics'|'plotter',><'xor'|'normal',>x,y)` draws a line (with attributes set by the `pen` command) from the current location (set by the `move` command) to the absolute location with coordinates `x` and `y`.

The `pen`, `move`, and `draw` commands below show two typical sequences of commands. In the first sequence, a yellow line is displayed on the graphics window at the `th` level.

1. `pen('graphics','yellow')`
   Select the graphics window and yellow as the active color
2. `move(wcmax-sc-wc,vp+th)`
   Move to left edge of chart as x and the threshold level as y
3. `draw(wcmax-sc,vp+th)`
   Draw a line to the right edge of the chart and at the threshold level as y

In the second sequence, two cursors are drawn on the plotter using pen 3.

1. `pen('plotter','pen3')`
   Select the plotter and pen 3
2. `move(wcmax-sc-wc*(cr-sp)/wp,-20)`
   Move to the cursor position along x and the bottom of the chart along y
3. `draw(wcmax-sc-wc*(cr-sp)/wp,wc2max)`
   Move to cursor position along x and to the top of the chart along y
4. `move(wcmax-sc-wc*(cr-delta-sp)/wp,-20)`
   Move to delta position along x and the bottom of the chart along y
5. `draw(wcmax-sc-wc*(cr-delta-sp)/wp,wc2max)`
   Move to delta position along x and the top of the chart along y

To draw a box on a plotter or a display, use

```
box(<'plotter'|'graphics',>x1mm,x2mm,y1mm,y2mm<,'nolimit'>)<
:r1,r2>
```

with the values for the left edge (`x1mm`), right edge (`x2mm`), bottom edge (`y1mm`), and top edge (`y2mm`) specified as arguments (e.g., `box(20,100,40,150)`. The location of the edges are given in plotter units (mm on most plots) and are scaled in mm for the graphics display. (If units are in Hz or ppm, you can use the `hztomm` command to convert to plotter units.) The keyword `'nolimit'` allows the box to extend outside the limits determined by the parameters `sc`, `wc`, `sc2`, and `wc2`.

Table 45 summarizes the commands for line drawing by the user.

Table 45. User-Controllable Line Drawing Commands

Commands	
`box*`	Draw a box on a plotter or graphics display
`draw*`	Draw line from current location to another location
`hztomm(x_position)<:xmm>`	Convert location from Hz or ppm to plotter units
`move(<'graphics'|'plotter'>,x,y)`	Move to an absolute location to start a line
`pen*`	Select a pen or color for drawing

```
* box(<'plotter'|'graphics',>x1mm,x2mm,y1mm,y2mm<,'nolimit'>)<:r1,r2>
  draw(<'graphics'|'plotter',><'xor'|'normal',>x,y)
  pen(<'graphics'|'plotter',><'xor'|'normal',>pen|color)
```

Chapter 10. Storing, Retrieving, and Moving Data

Sections in this chapter:

- 10.1 “Working with Directories and Files” this page
- 10.2 “Storing Data” page 277
- 10.3 “Retrieving Data” page 279
- 10.4 “Transferring Data Using Ethernet and limNET” page 281
- 10.5 “Converting Data Between Systems” page 286
- 10.6 “Magnetic Tape Operations” page 289
- 10.7 “Compressing Data” page 292

If you wish, you can do virtually all file and directory operations should through a series of interactive menus in the main menu system. These menus are accessible through the File button in the Main Menu or by entering the `files` command. Chapter 4, “Using the VNMR Menu System,” provides a complete description of the menus.

10.1 Working with Directories and Files

Typical operations with directories and files are saving and retrieving data, copying files, deleting and renaming files, and examining the contents of directories and files. This section covers the tools available for these operations. Table 46 lists these tools.

Default Directory

File names always assume the existence of a *default directory*, also called the *current working directory*. This is the directory the user currently is in. To display the path of the current working directory, enter the command `pwd`.

The default directory is set with the change directory command `cd<(directory)>`, where `directory` is the name of the new default directory; for example, entering `cd('/export/home/steve/vnmrsys')` changes the current working directory to the directory `/export/home/steve/vnmrsys`. Entering `cd` alone sets the current working directory to the user’s home directory (the tilde symbol “~”, shorthand for “the home directory of” in UNIX, does not work with VNMR commands).

By making the directory containing a file the current directory, file name entry is simplified. For example, if the default directory is set to `/vnmr/fidlib`, the file names `andro1.fid` and `/vnmr/fidlib/andro1.fid` are equivalent.

The `defaultdir` parameter holds the name of the default directory for the `files` menu system. Chapter 4, “Using the VNMR Menu System,” describes this menu.

Table 46. Directory and File Handling Commands and Parameters

Commands	
`cat(file1<,file2,...>)`	Display one or more text files in text window
`cd<(directory)>`	Change working directory
`copy(<'-r',>from_file,to_file)`	Copy a file
`cp(<'-r',>from_file,to_file)`	Copy a file
`delete(file1<,file2,...>)`	Delete file, parameter directory, or FID directory
`dir<(string)>`	List files in directory
`lf<(directory)>`	List files in directory
`ls<(directory)>`	List files in directory
`mkdir(directory)`	Create new directory
`mv(from_file,to_file)`	Move and/or rename a file
`pwd<:directory>`	Display current working directory
`rename(from_file,to_file)`	Move and/or rename a file
`rm(file1<,file2,...>)`	Delete file
`rmdir(directory)`	Remove directory
Parameters	
`curexp` {string}	Current experiment directory
`defaultdir` {string}	Default directory for the files menu system

Creating and Manipulating Directories

A new directory is created by the `mkdir(directory)` command. If a directory is no longer needed, the `rmdir(directory)` command removes one or more empty directories (i.e, the directory does not contain files). The `mv(old_name,new_name)` command renames a directory, and the `copy(old_name,new_name)` command makes a copy of the directory entered as the first argument (and all subdirectories and files of that directory). The new directory name is specified by the second argument.

The commands `lf`, `ls`, and `dir` list files in the current working directory on the text output window. If a directory is specified as an argument to `lf` or `ls`, the files in that directory are listed instead of the current directory. `dir` can include a string argument containing the same options as used with the UNIX `ls` command.

Creating and Manipulating Files

Files are typically created by data storage activities such as saving files, FIDs, or parameters. If a file is no longer needed, the `delete(file1<,file2,...>)` command removes a file from the file system. The `rm(file1<,file2,...>)` command also remove files, but `delete` is preferred because it is safer. `rm` functions like the powerful UNIX command of the same name and can inadvertently delete important files without warning, even for experienced users.

The `rename(old_name,new_name)` command changes the name of a file. By providing different directory paths as arguments, `rename` can also be used to move a file from one directory to another. The `mv(old_name,new_name)` command works the same as the `rename` command.

To make a copy of a file, enter the VNMR command `copy(old_name,new_name)` with the name of the file you want to copy as the first argument and the new name as the second argument. Include different directory paths for each file if you want to both copy the

file and, at the same time, move it to another directory. The command `cp(old_name,new_name)` works the same as the VNMR `copy` command.

To display the contents of one or more text files, use `cat(file1<,file2...>)`. The `cat` command places the text of each file, in the order given by the arguments, in the text window. If the text is longer than what one window can hold, `cat` pauses after the window has filled and waits for a keystroke from the operator to fill the window with more text.

The `curexp` parameter is useful when accessing text files generated by various commands. `curexp` contains the full UNIX path to the currently active experiment. For example, `cat(curexp+'/fp.out')` displays the contents of the `fp.out` file in the current experiment directory.

10.2 Storing Data

As explained previously, NMR data on the VNMR data system is acquired in a temporary disk file the known as an *experiment* and is identified by the file name `exp#`, where # is an integer from 1 to 9999, (e.g., `exp1` or `exp6`). Data reside in an experiment indefinitely until another set of data is collected in the same experiment. At some time, however, it is generally desirable to transfer the data to a more permanent file. The data can be transferred to a file on a hard disk, to a magnetic tape, or even via a mechanism, such as Ethernet, to some remote data system. Table 47 lists tools for storing data.

Table 47. Data Storage Commands and Parameters

Commands	
`autoname`	Create path for data storage
`svf<(file<,'nolog'><,'arch'>)>`	Save FIDs in current experiment
`svp(file)`	Save parameters from current experiment
`svs(file)<:status>`	Save shim coil settings
`writefid(file<,element_number>)`	Write numeric text file using a FID element
Parameter	
`shimspath` {string}	Path to user's shim directory

Experiment Files

An experiment such as `exp1` consists of one or more FIDs, one or more spectra, various parameters including nine "saved displays," a text file, and a number of other files. Because the FID is maintained separately from the spectrum, it is *not* necessary to save data permanently *before* performing the Fourier transform or other data processing.

In general, the recommended course of action using a VNMR data system is to save the data in a permanent file as the *last* action that you perform on the data. In this way, the result of operations performed during data processing (choice of weighting functions, referencing, phasing, scaling, etc) are preserved with the data, and should the data be recalled later, it will incorporate all of this information automatically.

Saving Data

Data are saved using the `svf<(file)>` macro. If a file name is not entered as an argument, `svf` asks for one. Only the FID is saved, not the spectrum, since the spectrum can always be reconstructed from the FID.

The `svf` macro creates a directory with the suffix `.fid` that contains the following four files, each with a special purpose:

- File `fid` contains the raw data (the FID).
- File `procpar` contains the parameters.
- File `log` contains the acquisition log.
- File `text` contains your annotations.

For arrayed experiments (containing multiple FIDs), `svf` saves all FIDs in a single file; there is no special command to allow individual FIDs of the array to be saved.

`svf` also saves the data files (`.def`) acquired with *GLIDE*.

If you place relevant information into the `text` file using the `text` command, it will be far easier to return to the data at some future time and understand exactly which experiment is stored in that particular file.

The command `writefid(file<,element_number>)` writes a text file using data from the selected FID element. The default for `element_number` is 1. The command writes two values per line. The first is the value from the X (real) channel, and the second is the value from the Y (imaginary) channel.

The `autoname` command creates file names from information in text files and from the values of VNMR parameters. It determines a path where data might be stored. `autoname` can be used in nonautomated sessions to generate a path name; it is used the same way that the `autoname` parameter is used during automation.

Saving Parameters

Parameters from the current experiment are saved by the macro `svp<(file)>`. A file with the `.par` suffix is created, which contains the parameters and text. If `svp` is entered without an argument, you are prompted for a file name. Unlike the `svf` macro, `svp` reflects any changes made in parameters up to the moment of entering `svp`, including acquisition parameters.

Saving Shim Coil Settings

All shim coil settings except Z0 are saved with the command `svs(file)`. If the name of the file entered as an argument is a relative path, `svs` looks for a `shims` subdirectory in the following order:

1. If the `shims` subdirectory exists in your VNMR user directory, `svs` stores shim coil settings there.
2. If the `shims` subdirectory does not exist, `svs` looks for a global parameter named `shimspath`. If `shimspath` is present, it is expected to contain the name of a directory. If this directory exists, `svs` saves the settings there if a new entry can be created.
3. If step 2 does not work, `svs` stores the shims in the `/vnmr/shims` directory (provided you have write permission).

If the name of the file entered as an argument is an absolute path, the file is saved directly.

10.3 Retrieving Data

At times, you need to recall stored data. Table 48 lists tools for data retrieval. The information in this section describes several methods for retrieving data in VNMR.

Table 48. Data Retrieval Commands and Parameters

Commands	
`compressfid(<indir,>outdir)`	Compress double-precision VNMR FID data
`compressfid*`	Compress double-precision VNMR FID data (UNIX)
`makefid*`	Make a FID element using numeric text input
`parfix`	Update parameter sets
`rt<(file<,'nolog'>)>`	Retrieve FIDs
`rtcmx<(file)>`	Retrieve Spinsight data into current experiment
`rtp<(file)>`	Retrieve parameters
`rts(file)<:status>`	Retrieve shim coil settings
`rtv*`	Retrieve individual parameters
`updatepars`	Update all parameter sets saved in a directory

`* compressfid –i indir –o outdir –f`
`compressfid –e exp_number –o outdir –f`
`makefid(file<,element_number><,format>)`
`rtv<(file,par1<,par2,...>)><:variables>`	

Parameter	
`parversion` {real value}	Version of parameter set

Using rt, rtp, and rts to Retrieve Files

The macro `rt<(file)>` retrieves FIDs stored in the FID file `file.fid` into the current experiment (e.g., `rt('/vnmr/fidlib/fid1d')`). If `file.fid` does not exist and the parameter file `file.par` does exist, `rt` retrieves the parameters only from `file.par`. If `rt` is entered without an argument, it asks for a file name. In that case, the file name can be given without single quotes.

Retrieved data is placed into the current experiment. Any data in that experiment is overwritten. Remember that it is the FID that is retrieved and it must be transformed, but if the data is stored *after* it is originally processed, as previously recommended, it is not necessary to rephase, re-reference, or otherwise reprocess the data, except as desired.

The macro `rtp<(file)>` retrieves all parameters from the parameter file `file.par`, if this file exists. If not, and if `file.fid` *exists*, `rtp` retrieves the parameters only from the FID file `file.fid`. If you only wish to retrieve a few parameters from a file stored with `svf` or `svp`, enter the command `rtv<(file,par1<,par2,...>)>` with the file name and one or more parameter names as arguments. If `rtp` or `rtv` are entered without an argument, you are prompted for a file name. In that case, the file name can be given without single quotes.

To retrieve shim settings, the command `rts(file)` locates a preexisting file of shim settings saved by the `svs` command and copies the settings into the current parameter set of the current experiment. If the file name entered as an argument is a relative path, `rts` looks for a `shims` subdirectory in the following order:

1. If `shims` exists in your VNMR user directory, `rts` copies the settings.
2. If the `shims` subdirectory does not exist, `rts` looks for a global parameter named `shimspath`. If it is present, `shimspath` is expected to contain the name of a

directory. If this directory exists, `rts` copies the settings if it locates the requested file.

3. If step 2 does not work, `rts` tries to locate the file in `/vnmr/shims`.

If the name of the file entered as an argument is an absolute path, the file is located directly. A message is displayed at the end about the success or failure of `rts`.

To retrieve Spinsight data into the current experiment, use the `rtcmx<(file)>` command.

Using *GLIDE* to Retrieve Data

GLIDE can also be used to retrieve data. However, use this method to retrieve only data on parameters and FIDs. Perform the following steps to retrieve data with *GLIDE*:

1. Activate *GLIDE* by clicking GLIDE button in the Permanent menu.
2. Click on Recall.
3. In the Recall Setup window, type the full path of the FID file that you want.
4. Click on Retrieve.

   The data file is recalled. If the data was acquired with *GLIDE*, the `.def` files are also recalled into *GLIDE*.

Using CDE File Manager to Retrieve Data

The CDE File Manager can be used to retrieve data on parameters, FIDs, or shim files. To use this method, the `listenon` macro must be, or must have been, executed. If file retrieval is a regular mode of operation, consider putting `listenon` in your local `login` macro. Do the following steps to retrieve data with CDE:

1. Start the CDE File Manager from the CDE toolbar.
2. Go to the desired directory and double-click the desired parameter, FID, or shim file.

   After you have selected the desired FID file, it is processed and displayed. `.def` files (files acquired with *GLIDE*) are retrieved into *GLIDE*.

Correcting Saved Parameter Sets

The `updatepars` macro corrects saved parameter sets. With the release of VNMR version 4.2, all the parameters, upper limit, lower limit, and step sizes were tightened. Further additions were made in VNMR 4.3 and VNMR 5.3. `updatepars` searches a directory for parameter and FID files, and corrects the `procpar` files found. It is recommended that the user execute this macro on all older parameter sets before using the parameter set again. `updatepars` overwrites parameters in the current experiment. The corrections that are applied to the parameter sets are defined by the `parfix` macro. When a parameter set is updated with `updatepars` or `parfix`, the parameter `parversion` is set to 5.3 to indicate the version. The `updatepars` macro uses the current experiment to process the parameter sets. Therefore, whichever experiment is chosen for running `updatepars` should not contain a valuable data set.

User-Written FID Files

The `makefid(file<,element_number><,format>)` command lets you introduce computed data into an experiment by creating a FID file. To use this command, you must give the name of a file with input as the first argument. This file must contain numeric values, two per line. The first value is assigned to the X (or real) channel; the second value on the line is assigned to the Y (or imaginary) channel.

The other two arguments can be entered in any order: `element_number` is the number of the element or FID (the default is the first element or FID), and `format` is a string with the precision of the resulting FID file (the default is `'32-bit'` for double-precision data). Before using `makefid`, read the description of it in the *VNMR Command and Parameter Reference* for further details.

10.4 Transferring Data Using Ethernet and limNET

One of the most efficient mechanisms for transferring data from one location to another is over an Ethernet network. Ethernet can be used to transfer data, and hence to store and retrieve data remotely, on a wide variety of systems, including VNMR systems (*MERCURY-VX*, *MERCURY*, UNITY*INOVA*, UNITY*plus*, *GEMINI 2000*, UNITY, and VXR-S), VXR-style systems (Gemini, VXR-4000, and XL), and VAX computers.

Ethernet encompasses a number of ideas, but for our purposes here only hardware and software (or "protocol") is considered. On the hardware side, Ethernet is a standard feature of the VNMR data system (Ethernet hardware is optional on VXR-style systems). On the software side, VNMR includes standard UNIX software using the Internet Protocol (IP) that enables data transfer between one VNMR system and another, or between a VNMR system and other computers supporting IP.

VNMR software includes a proprietary Ethernet protocol named limNET™ (Laboratory Information Management Network, a Varian trademark). This protocol is required for exchanging information with VXR-style systems, on which only the limNET protocol is supported. The limNET protocol is also available for VAX and IBM RS/6000 computers, where it is used to transfer data from VXR-style systems.

Table 49 lists commands associated with data transfer over Ethernet and limNET.

Table 49. Ethernet and limNET Data Transfer Commands

Commands	
`dnode`	List valid limNET nodes (VNMR,UNIX)
`eaddr`	Display Ethernet address (VNMR,UNIX)
`elist(remote_mode,remote_dir)`	List directory of remote system (VNMR)
`elist remote_mode remote_dir`	List directory of remote system (UNIX)
`eread*`	Transfer file from a remote source (VNMR)
`eread*`	Transfer file from a remote source (UNIX)
`ewrite*`	Transfer file to a remote destination (VNMR)
`ewrite*`	Transfer file to a remote destination (UNIX)
`* eread(local_file,remote_node,remote_file)`	`(VNMR)`
`eread local_file remote_node remote file`	`(UNIX)`
`ewrite(local_file,remote_node,remote_file)`	`(VNMR)`
`ewrite local_file remote_node remote_file`	`(UNIX)`

Transferring Data Using Ethernet

UNIX commands `ftp` (file transfer program) and `rcp` (remote copy program) are among the commands available to transfer of files from one VNMR system to another using Ethernet. These commands are not supported inside VNMR, although a macro can easily be created if this is desirable.

Since most FID files in the VNMR file system are stored as directories, the `rcp` program is probably the most useful, because it can transfer entire directories, not just individual files. The structure of `rcp` is identical to that of the standard UNIX `cp` program, except that the remote file name must be preceded by the name of its computer (the remote host-name) followed by a colon. The following two examples should suffice:

- Remote copy of an entire directory (`-r` option) in the current directory named `noesy.fid` (data files always end in `.fid`) to a remote host (VARIAN600) into the named file: `rcp -r noesy.fid VARIAN600:/usr2/slp/noesy.fid`
- Remote copy of a `newfid.fid` in the home directory of `vnmr1` on the remote host (VARIAN500), into the home directory of `vnmr1` (where it will be given the same name): `rcp -r VARIAN500:~vnmr1/newfid.fid ~vnmr1`

The names of the known remote hosts are contained in the file `/etc/hosts` or in the NIS files (enter `ypcat hosts` in a UNIX shell) and are established by the system administrator. A user only needs to know the name of each computer system. To test connectivity, the `rsh` command is available (e.g., `rsh VARIAN500 ls`).

Transferring Data Using limNET

The user interface to the limNET software consists of the commands `eread`, `ewrite`, `elist`, `dnode`, and `eaddr`. These commands are available from the VNMR program or from the UNIX shell. In VNMR, each argument is a string, so typically each argument must be enclosed in single quotes, although string variables can be used also. From the UNIX shell, each argument is separated by a space. Examples of both are given below. Throughout the section, VXR-style (Gemini, VXR-4000, or XL) systems are usually referred to as a *remote node*. Note that after data is transferred, it must be converted. This is covered in “Converting Data Between Systems” on page 286.

To Display Remote Nodes Available

The `dnode` command displays all remote nodes available to limNET. `dnode` is entered without arguments and can be used from either VNMR or the UNIX shell.

To Transfer a File From a Remote Node

The `eread` command transfers the contents of a file associated with a remote node to the local destination. The syntax is the following:

From UNIX: `eread local_file remote_node remote_file`

From VNMR: `eread(local_file,remote_node,remote_file)`

All three arguments are required. The names of the remote computers or *nodes* available to the limNET protocol are held in the `/vnmr/nodes` file. The `dnode` command displays a list of available nodes, which each user needs to know.

For example, to transfer the contents of the file `dsk1.osv700`, which resides in the remote node called `v400`, to the local destination file called `osv700`, enter:

From UNIX:	`eread osv700 v400 dsk1.osv700`
From VNMR	`eread('osv700','v400','dsk1.osv700')`

To Transfer a File To a Remote Node

The `ewrite` command transfers the contents of a local file from a UNIX system to the remote destination file associated with the remote node. The syntax is the following:

From UNIX:	`ewrite local_file remote_node remote_file`
From VNMR:	`ewrite(local_file,remote_node,remote_file)`

The arguments are defined the same as for the `eread` command.

To List the Contents of a Directory on a Remote Node

The `elist` command displays a listing of the contents of a directory on a remote VXR-style system. The syntax is the following:

From UNIX:	`elist remote_node remote_dir`
From VNMR:	`elist(remote_node,remote_dir)`

where `remote_dir` is the name of the directory on the remote system.

For example, entering from UNIX
`elist gemini fidlib`

`or entering from VNMR`
`elist('gemini','fidlib')`

provides a list similar to the following:

```
APT         DR      5       45
HETCOR      DR      5       141
C13         DR      5       45
DEPT        DR      5       144
H1          DR      5       23
COSY        DR      5       141
```

The contents are listed in the order they appear in the remote directory.

To Display Local Node Address

The `eaddr` command address of your local node. This command is entered without arguments and can be used from either VNMR or the UNIX shell.

File Suffixes

Whenever limNET is used to transfer a file from a VXR-style (Gemini, VXR-4000, or VXR) system to a UNIX-based VNMR (*MERCURY-VX*, *MERCURY*, UNITY*INOVA*, UNITY*plus*, *GEMINI 2000*, UNITY, or VXR-S) system, a suffix is appended to the UNIX file name by the VNMR system. This lets other software on the VNMR system know what type of VXR-style file the UNIX file represents.

Similarly, when limNET is used to transfer a file from a VNMR system to a VXR-style system, the VNMR system uses a suffix to determine what kind of VXR-style file the file represents. If the UNIX file name contains no suffix or is ambiguous, the limNET software assumes the file is a VXR-style data file.

The limNET protocol can transfer VXR-style directories, program files, and data files. (The VXR-style commands `DIR` and `DLIST` use the mnemonics `DR`, `PR`, and `DA`, respectively, to identify such entries.) The VNMR suffix for each is the following:

- Directory files have the .### suffix (see below).
- Program files have the `.prg` suffix.
- Data files have the `.dat` suffix.

The suffix for a directory file is the total number of entries allocated in the VXR-style directory. Therefore, if `FIDLIB` has (e.g., 36 entries, it becomes `fiblib.36` in VNMR). For program files and data files, a dot and `prg` or `dat` is added; (e.g., `MNPPGM` becomes `mnppgm.prg` and `VCOEFS` becomes `vcoefs.dat`).

Be aware that the information in the I2 field (normally the date) is lost when the file is transferred to VNMR. The exception is, of course, a VXR-style directory.

Initiating Transfers from a Remote Node

The limNET software lets you start a transfer from a remote node on a VXR-style system. When you use the `ewrite` command to transfer a file to a UNIX system, the name of the file on the UNIX system will have a suffix indicating what type of VXR-style entry the original file was.

When you use the `eread` command to transfer a file from a UNIX system, the limNET software on the UNIX system searches for the file as specified in the original `eread` command. If a file is found, limNET on the UNIX system will transfer it to your local VXR-style system. If no file is found, limNET checks if any files have the original name with the suffix added. If exactly one such file is found, it is transferred to your local VXR-style system. In either situation, the type of entry on the local VXR-style system is based on the suffix of the file on the remote system. If the remote file has no suffix or the suffix is ambiguous, the entry type defaults to a data file.

No upper-case characters can appear in either the directory or the file name on the UNIX system. If any are used, the transfer fails with a report indicating the file does not exist or cannot be found. The limNET software converts any upper-case letters to lowercase when accessing the file system of UNIX.

File security on the UNIX computer is maintained several ways. The limNET server insists that the world have permission to complete the requested transfer. Thus, a file can be read only if the world has read access to that file. Read and execute access is also required for the parent directory, and each level above it, all the way back to the root. For example:

File to be read	*Required access*
`/export/home/vnmr1/vxr/example`	`rwxr–xr––`

Parent directories	*Required access*
`/export/home/vnmr1/vxr`	`rwxr–xr–x`
`/export/home/vnmr1`	`rwxr–xr–x`
`/export/home`	`rwxr–xr–x`

/export	rwxr–xr–x
/	rwxr–xr–x

If /export/home/vnmr1 does not have execute or read access for the world set, then the file /export/home/vnmr1/vxr/example is not accessible from limNET, even if its file protection does allow world access. Also, no entry can be overwritten or erased, even if the file protection would allow it.

A new file can be written only if the world has read, write, and execute access to the parent directory. Read and execute access is required for each directory above the parent in the tree; for example:

File to be written	*Required access*
/export/home/vnmr1/limnet/newfid.5	N/A (to be created)

Parent directories	*Required access*
/export/home/vnmr1/limnet	rwxrwxrwx
/export/home/vnmr1	rwxr–xr–x
/export/home	rwxr–xr–x
/export	rwxr–xr–x
/	rwxr–xr–x

A good idea is to create a separate directory for limNET transfers so write access for the world can be limited to that subdirectory.

Error Messages from limNET

The dnode and eaddr commands should never produce an error. If one occurs, contact the system administrator because the limNET software was probably not installed correctly. The eread and ewrite commands can fail for a variety of reasons. Some of the error messages that may appear are listed below in alphabetical order with an explanation of each message and the recommended action:

Can't open limNET service file

The limNET server was never started. Contact the system administrator.

Error connection to public socket: Client connection refused

The limNET server is no longer functioning.

error obtaining internet host name

The file /etc/hosts is not present or does not contain the address of the local node.

ether_hostton failure: no such file or directory

The file /etc/ethers is not present (version 2.0 of limNET only). This message is produced by the eaddr command and the limNET server.

Incorrect number of arguments

Use exactly three arguments for eread and ewrite, as described above.

Network timeout

The local system software found the address of the remote node and attempted to send it a request, but failed to receive a response. This can occur if the remote node does not have limNET installed, if the node is down or otherwise disabled, if the Ethernet address for the

remote node is wrong, if the Ethernet hardware has not been installed or configured correctly, of if the local node is not physically connected to the network.

If this error message is a result of a read or write transfer initiated from a VXR, Gemini, or XL host, the cause might be that the destination directory does not have read or write permission set for the world.

Public socket connect error: Network unreachable
Public socket connect error: Connection refused

Either one of these messages indicates that the local host is not connected to the Ethernet hardware. In this situation, the system administrator must terminate the limNET server, connect the local node to the network, and then restart the server.

The system administrator can stop the limNET server by taking the following steps:

1. Enter the UNIX command `ps-e` on Solaris to find the process ID of the limNET server. The name of the process is `limnetd`.
2. Enter the UNIX command `kill –a PID`, where `PID` is the process ID of the limNET server. Only `root` can execute this `kill` command.

Remote host busy

The remote node is currently involved in another limNET transfer. The VXR-4000 system allows only one transfer at a time. Try the command again in a few minutes.

Remote node not found

The `remote_node` argument could not be located in the node file.

10.5 Converting Data Between Systems

Files transferred from VXR-style systems (Gemini, VXR-4000, or XL) or Bruker systems are in a format that must be converted to a usable format for VNMR and then stored for later use.

- For all text files, the `unix_vxr` and `vxr_unix` commands convert the files between VNMR and VXR-style systems.
- For VXR-style system data files, the `convert` command makes the transferred data usable for VNMR and `decomp` breaks up transferred libraries and stores the files in a VNMR subdirectory.
- For Bruker data files, the `convertbru` and `sread` commands convert the Bruker data and read the converted data into VNMR.

Table 50 summarizes the commands used for data conversion.

Converting Text Files

Text files have a different format (the byte order is reversed) on the UNIX-based systems than they do on VXR-style systems. To enable moving text files, such as pulse sequences, from one system to another, the following commands with the file names as arguments perform a format conversion.

The syntax for UNIX text to VXR-style text:

From VNMR:	`unix_vxr(UNIX_file,VXR_file)`
From UNIX:	`unix_vxr UNIX_file VXR_file`

Table 50. Data Conversion Commands

Commands	
`convert(VXR_file)`	Convert data set from VXR-style system
`convertbru(file<,options>)`	Convert Bruker data (VNMR)
`convertbru file <options>`	Convert Bruker data (UNIX)
`cpos_cvt VXR_file`	Convert data set from VXR-style system (UNIX)
`decomp<(VXR_file)>`	Decompose a VXR-style directory
`sread(file<,template>)`	Read converted Bruker data into VNMR
`unix_vxr(UNIX_file,VXR_file)`	Convert UNIX text files to VXR-style (VNMR)
`unix_vxr UNIX_file VXR_file`	Convert UNIX text files to VXR-style (UNIX)
`vxr_unix(VXR_file<,UNIX_file>)`	Convert VXR-style text files to UNIX (VNMR)
`vxr_unix VXR_file UNIX_file`	Convert VXR-style text files to UNIX (UNIX)

The syntax for VXR-style text to UNIX text:

From VNMR:	`vxr_unix(VXR_file<,UNIX_file>)`
From UNIX:	`vxr_unix VXR_file UNIX_file`

In using this syntax, `VXR_file` cannot be the same as `UNIX_file`.

Do not use `vxr_unix` on a file other than a text file obtained from a VXR-style-based system. The VNMR command `vxr_unix` only may omit `UNIX_file`, in which case the output is sent to the text window.

Converting Data Files

Data files also have a different format on the UNIX-based systems than they do on the VXR-style systems. Data files transferred from a VXR-style system therefore have to be converted to the format used in UNIX-based systems.

From VNMR, the command `convert(VXR_file)` loads the data from the file `VXR_file` into the current experiment and converts it to the new format (the `convert` command must be used instead of `rt` when VXR-style data is to be read).

A similar UNIX command, `cpos_cvt VXR_file`, also converts the data set but writes the converted data into a subdirectory of the current working directory, using the original name of the data set.

Decomposing a Library

The command `decomp<(VXR_file)>` takes a VXR library, as loaded from a VXR-style system, and extracts each entry into a separate UNIX file. The file can be obtained from a magnetic tape or over limNET. A limit of 432 entries is imposed. `decomp` creates a UNIX subdirectory in the current working directory and uses that to write each VXR entry as a UNIX file. The name of the UNIX subdirectory is derived from the VXR library name. The name of the original VXR file must have an extension in the form `.NNN`, where `NNN` is the number of entries in the original VXR library (limNET automatically supplies this extension).

Note that when data is copied from a VXR-style system, all files should first be stored in a directory on the system and then stored on the tape as one file (or transferred over Ethernet as one file). Otherwise, the command `decomp` will not work.

Step-by-Step Example with limNET

The VNMR command `convert` takes the FID file from a VXR-style (Gemini, VXR, or XL) system into a format with which the VNMR program can work. The reverse capability, converting data from VNMR format into VXR-style format, does not exist. The example below shows the interaction on a Sun system using limNET with the remote VXR-style system, a Gemini named "gemini."

1. The following commands are entered with the responses shown:
```
> eread h1 gemini fidlib.h1
23
> ls h1*
h1.5
> vnmr
```
2. VNMR starts up. In VNMR, enter: `convert('h1.5')`

   The `convert` command works with the output from the VXR-style command SVF. An output of "`23`" from the `eread` command indicates the file `fidlib.h1` is 23 blocks in size. The suffix "`.5`" appears because the entry `h1` is a VXR-style directory with 5 entries, as is typical for saved FIDs on VXR-style systems.
3. To save the data in VNMR format, enter: `svf('h1')`
4. Verify the operation was successful by entering `ls('h1/*')`

   VNMR displays the contents of the directory `h1.fid`, created by the `svf` macro:
```
fid     procpar     text
```

The `decomp` program takes apart libraries brought over from a VXR-style system. It creates a subdirectory on the UNIX system, using the name of the VXR-style library, and then it copies each entry in the VXR-style library to a separate file in that subdirectory. The next example uses the setup above with the `convert` command.

1. The following commands are entered, with the responses shown:
```
> eread fidlib gemini fidlib
64   128   192   256   320   384   448   512   540
> ls fidlib*
fidlib.36
> decomp fidlib.36
Loading fidlib/apt.5, 45 blocks
Loading fidlib/c13.5, 45 blocks
Loading fidlib/cosy.5, 141 blocks
Loading fidlib/dept.5, 144 blocks
Loading fidlib/h1.5, 23 blocks
Loading fidlib/hetcor.5, 141 blocks
> ls fidlib
apt.5   c13.5   cosy.5   dept.5   h1.5   hetcor.5
>
```
2. At this point, any of the VXR-style FIDs `apt.5`, `c13.5`, `cosy.5`, `dept.5`, and `h1.5` can be converted into VNMR format using the VNMR `convert` command (e.g., `convert('fidlib/c13.5')`). Note that here the subdirectory `fidlib` is included as part of the `convert` command.

In normal operation, the `decomp` program is not used with the actual VXR-style FID files, such as `h1.5`. If for some reason the actual data is to be examined using a separate program, the `decomp` program would then be suitable.

Converting Bruker Data

The command `convertbru(file<,options>)` converts 32-bit Bruker AMX data and 24- and 32-bit Bruker AM data into a 32-bit format compatible with Varian's `sread` program. The `file` argument to `convertbru` is the name of the input argument. From UNIX, the syntax is `convertbru file options`. Refer to the *VNMR Command and Parameter Reference* for detailed information on `convertbru`, including the options available and examples.

After converting the Bruker data into the new format, the converted data can be read into VNMR using the command `sread(file.cv'<,template>)`, where `file` is the name of the file containing the converted data and `template` is the full path of a parameter template file (do not append `.par` to the file name)—for example, `sread('brudata.cv','/vnmr/parlib/bruker')`. The name of the file containing the parameter template is optional; the default is `bruker.par`. If no parameter template is specified and `bruker.par` cannot be found in the user or system `parlib` directory, `sread` aborts with an appropriate error message.

10.6 Magnetic Tape Operations

Table 51 lists UNIX and VNMR commands associated with magnetic tape operations.

Table 51. Magnetic Tape Operations Commands

Commands	
`dd <option=value>...`	Convert and copy a file (UNIX)
`mt <-f tape> command... <count>`	Magnetic tape control (UNIX)
`readbrutape file <num_skipped>`	Read Bruker data files from 9-track tape (UNIX)
`tape(<type,>option<,file1,...>)`	Read tapes from VXR-style system (VNMR)
`tape <type> <option> <file1>`	Read tapes from VXR-style system (UNIX))
`tar <options>`	Create tape archives, add or extract files (UNIX)

The simplest technique to operate the tape unit is to use the interactive tape file handling menu described in "File Menus" on page 87. This menu lets you perform all relevant operations: reading files from tape, writing files to tape, and listing a tape catalog.

The second method is to use the UNIX command `tar` (tape archive). Run in a separate window from VNMR, a `tar` backup can proceed completely as a separate process. If you have many megabytes of data to back up, there is no reason to tie up VNMR with this process. Simply open a separate window and use `tar`.

A number of ways are available for reading from and writing to a streaming tape. See the documentation of the UNIX `tar`, `mt`, and `dd` commands for some possibilities. For example, on systems using Solaris, the following commands append files `abc` and `xyz` to an already used tape:

```
mt –f /dev/rmt/0lbn rew
mt –f /dev/rmt/0lbn fsf 1
tar cvf /dev/rmt/0lbn abc xyz
mt –f /dev/rmt/0lbn rew
```

If data is written onto a magnetic tape using a Sun or IBM RS/6000 computer and is then to be copied into a Silicon Graphics computer, the byte order on the tape is reversed. To read such a tape you must use the `/dev/tapens` device when using `tar`:

```
tar xvf /dev/tapens
```

If data has been written onto a magnetic tape on a Silicon Graphics computer and is to be copied back onto a Sun or IBM RS/6000 computer, the byte order is again reversed. The `tar` command cannot be used alone in this case; instead, use the command string:

```
dd if=/dev/rmt/0lb conv=swab bs=20b | tar xvBfb - 20
```

(Note there is a space between the "`-`" and the "`20`" at the end of the command string.)

CAUTION: **Keep magnetic tapes away from the magnet. Data stored on the tape can be damaged by the strong magnetic field.**

Reading Tapes from Gemini, VXR-4000, and XL Systems

The command `tape(<type,>keyword<,file>)` displays the contents of a VXR-style tape (used on a Gemini, VXR-4000, or XL system), for use on a UNIX-based system, or reads one or files from a VXR-style tape into the current directory. `type` is the type of tape to be accessed (default is the 1/4 in. tape), `keyword` can be `'help'` (display entry options), `'cat'` (display catalog of files on tape), `'read'` (read file given by `filename`, maximum of four file names can be specified), `'rewind'` (rewind tape, 1/2 in. tape only), or `'quit'` (release the tape drive, 1/2 in. tape only).

If you are using VnmrI on an IBM RS/6000 computer or VnmrSGI on a Silicon Graphics computer, tapes from VXR-style systems can be read using the UNIX `dd` command. For the IBM RS/6000, the following command is appropriate:

```
dd if=/dev/rmt1 fskip=1 of=xyz.288
```

where `xyz` is the name of the directory you wish to create and 288 is the number of entries that were found in the Gemini or VXR directory (288 would correspond to a disk backup). The device can be something other than `rmt1`, such as `rmt0`.

For Silicon Graphics systems, the following commands are appropriate:

```
mt rewind
mt fsf 1
dd if=/dev/nrtape of=xyz.288 ibs=512000 conv=swab
mt rewind
```

In these commands, `xyz` is the name of the directory you wish to create and 288 is the number of entries that were found in the Gemini or VXR directory (288 would correspond to a disk backup).

For either system, the directory that results (`xyz.288` in this example) must next be decomposed by entering (e.g., `decomp xyz.288`).

The `decomp` command creates a new directory `xyz`, and the individual files found in that directory can be read into VNMR using the `convert` command.

Reading Bruker Data Files from 9-Track Tape

The UNIX shell script `readbrutape` reads one file from a Bruker tape into a UNIX file. The syntax used is `readbrutape file <number_skipped>`, where `file` is the name of the file read into UNIX. For identification, the `.bru` extension is added to the file name. The optional argument `number_skipped` is the number of files skipped and includes the header file, which is assumed to the first file on the tape. The default is the script reads the first file after the header file. If `number_skipped` is set to 0, there is no rewinding and the first file (or the next file) on the tape is read.

After running `readbrutape` to read the data file, it must be converted using the `convertbru` and `sread` commands for use with VNMR.

Sharing a Tape on a Network

A single tape can easily be shared between two or more computers, provided the systems are installed according to the instructions on remote installation in the manual *VNMR and Solaris Software Installation*. Files can be backed up or restored remotely over the network using the following UNIX commands:

- To read a tape catalog of a remote tape on a remote computer named “lal600”:
  `rsh -n lal600 dd if=/dev/rmt/0lb bs=20b | tar tvfbB - 20`
- To read all files from the remote tape:
  `rsh -n lal600 dd if=/dev/rmt/r0lb bs=20b | tar xvfbB - 20`
- To read named files (`file1`, `file2`, ...) from the remote tape:
  `rsh -n lal600 dd if=/dev/rmt/r0lb bs=20b | tar xvfbB - 20 file1 file2 ...`
- To write named files (`file1`, `file2`, ...) to the remote tape:
  `tar cvfb - 20 file1 file2 ... | rsh lal600 dd of=/dev/rmt/0lb obs=20b`

Unfortunately, the slightest error in typing one of these rather complex commands can make it go wrong. If you need to do this regularly, you should make up several shellscripts to accomplish the task in a simpler fashion. For more information, refer to documentation on the UNIX `tar` command.

Moving Data to PCs and Macintoshes via Floppy Disk

The 1.44-Mbyte floppy disk drive found on most SPARCstation computers provides a convenient way not only to store data but also to move data, particularly text files, between the Sun, PC and, Macintosh platforms.

The Sun command `fdformat` formats a 1.44-Mbyte floppy disk and allows it to be addressed as `/dev/rfd0`, a “raw” device. The floppy now acts like a tape and can be written to with the `tar` or `bar` commands. This method is ideal for open-access type instruments and provides a convenient way to share files between remote coworkers.

If you insert a floppy disk in the drive and format it using `fdformat -d`, a DOS file system is installed on the floppy disk. You can make the floppy known to the system by mounting the file, *provided no programs are running*.

If `volmgt` is not running, you can mount the file by logging in as `root`, then entering `mount -F pcfs /dev/diskette0 /pcfs`.

Now you can copy files to the `/pcfs` directory. For text files, you would enter `unix2dos Suntextfile DOStextfile`, which performs the necessary text conversion. At this point, after you enter the command `umount /pcfs` followed by the command `eject floppy` to remove the disk from the drive, you can take it directly to a PC and read the files (especially the text files). The only catch in all of this is that you have to be `root` to run these commands.

(Mac operating systems earlier than 7.5) To read this disk on a Macintosh, use one of the standard Mac-to-PC connectivity programs. With most of these programs, you can look at the disk contents on your desktop and automatically translate text files (basically stripping out line feeds) so you can read them.

Mac OS 7.5 and later can read a PC floppy disk without additional software.

You can also use the floppy disk as a UNIX file system:

1. After entering `fdformat` to format the floppy, enter:

```
newfs /dev/rfd0c
```

Alternatively, you can avoid the usual 10 percent "free space" in the file system from the command above by entering instead:

```
newfs -m 0 /dev/rfd0c
```

2. Create a directory and mounting point by entering:

```
mkdir /floppy
mount /dev/fd0c /floppy
```

Now `/floppy` is just a normal file system that you can read and write to.

3. When done with the floppy, enter:

```
umount /floppy
```

4. To insert a floppy with data already on it, insert it into the drive and enter:

```
mount /dev/fd0c /floppy
```

There is no need to reformat or create a new file system).

Sun has an unofficial method to get around the fact that only `root` has the privileges to do all of the above. In this method, `root` carries out each of the following steps:

1. If using Solaris, create a shellscript `mountfloppy` like this:

```
#! /bin/csh -b
mount –F pcfs /dev/fd0c /floppy
```

If not using Solaris, the shellscript `mountfloppy` is slightly shorter:

```
#! /bin/csh -b
mount /dev/fd0c /floppy
```

2. Create another shellscript `ejectfloppy` like this:

```
#! /bin/csh -b
umount /floppy
eject
```

3. Run a `chmod 4755` on the two shell scripts and then create a `/floppy` directory with 777 characteristics.

The user now uses `mountfloppy` and `ejectfloppy` in place of the `mount` and `eject` commands to accomplish the otherwise forbidden tasks.

10.7 Compressing Data

A number of data compression programs are available to reduce the space occupied by data on storage devices and to increase the throughput of data sent electronically. The standard UNIX `compress` utility is a general-purpose program that can compress any file, typically by 40 to 50 percent. The `compressfid` command is a more specialized program that is used to compress double-precision VNMR FID data to single precision.

Compressing and Uncompressing FID Data Files

If you enter `compress` with a file name (e.g., `compress mydata.fid`) from UNIX, the `compress` program replaces the file you specified with a compressed file and identifies it by adding a `.Z` suffix (e.g., `mydata.fid.Z`).

You can not do this on a directory, so to make this work on data you must compress the FID file itself. An easy way to accomplish this is to create a pair of macros. The first macro saves the compressed FID:

```
"svcf - save compressed fid"
svf($1)
shell('compress'+$1+'.fid/fid &')
```

The second macro retrieves the compressed FID:

```
"rtcf - retrieve compressed fid"
shell('uncompress'+$1+'.fid/fid')
rt($1)
```

Because `compress` does not work on directories, and because many files are often linked to one another, it is useful to combine various data files into a single (but separable) file. A simple mechanism to do this is to use the `tar` command to write not to a tape but to a file (e. g., `tar cvf mydata.fid.tar mydata.fid)`

This creates a new file `mydata.fid.tar` that is just a single file. Compress this file by entering `compress mydata.fid.tar`. The file `mydata.fid.tar.Z` is created.

To reverse the process, uncompress the file by entering:

```
uncompress mydata.fid.tar
tar xvf mydata.fid.tar.
```

This extracts files from the compressed file and makes it back into a directory.

Performing this process on the entire `/vnmr` directory, for example, creates a single file of 5.4 MB, compared to 11.9 MB for the complete directory, a 55 percent compression. This is an excellent way to cut down on disk and tape usage.

Compressing Digitally Filtered FID Files

Compressing digitally filtered (DSP) FID files creates two potential problems:

- DSP can produce a significantly higher dynamic range (depending on the amount of oversampling) and larger absolute numeric values than the equivalent FIDs acquired without DSP.
- Inline DSP produces FIDs in floating point format.

Because the UNIX compression of standard FIDs (using `compress` or `gzip`) largely relies on removing leading zeroes in those parts of the FID containing small numbers, the larger numbers alone will cause `compress` or `gzip` to be much less efficient (`gzip` is a public domain program available from the user library). And the bit pattern from floating point data is much less compressible than integer data because the floating point format contains fewer repetitive bit patterns. It is possible that the size of the file actually increases after applying the compression program.

If `compress` and `gzip` both do not work, the only compression option is the VNMR command `compressfid`, which forces a data set into single precision (`dp='n'`) format. A disadvantage of `compressfid` compared to `compress` and `gzip` is that the original data cannot be reconstructed after the `compressfid` compression, even though the information losses may be marginal in most cases.

Compressing Double-Precision VNMR FID Data

The command `compressfid` compresses double-precision VNMR FID data to single precision and updates the parameter `dp` in `procpar`. This results in a major decrease of almost 50 percent in the required disk space to store the data and a slight decrease in the resolution of the stored data. `compressfid` can be run through a macro interface in VNMR or directly at the UNIX level. For details, refer to the description of `compressfid` in the *VNMR Command and Parameter Reference*.

Glossary

acquisition computer — Computer in NMR system console that controls the acquisition process.

ADC — Analog-to-digital converter. Digitizes the analog signal from the probe.

Analog*Plus* filter — Type of real-time digital filter with similar characteristics to traditional analog filters, but uses digital technology to obtain flatter passband and sharper cutoff in the stopband compared to the corresponding analog filter.

array — Set of data that are related so they can be treated as a single entity.

Bayes software — Optional software available from Varian that uses Bayesian probability theory to directly analyze 1D, time-domain data, providing signal amplitude, frequency, and linewidth for all statistically significant resonances

Brickwall filter — Type of real-time digital filter with much sharper cutoff than the Analog*Plus* digital filter.

CDE — Common Desktop Environment. A UNIX windowing environment.

depth indicator — Device provided to position the sample accurately.n

diffusion software — Optional software available from Varian containing acquisition and analysis programs for the determination of diffusion constants using the pulsed gradie3nt echo method.

digital signal processing (DSP) — Capability of VNMR software to oversample the data, apply a digital filter to the FID, and then downsample the data. Benefits of DSP include constant noise level across the spectrum, improved integral accuracy, increased dynamic range, and flatter baselines.

downsampling — Reducing the number of data points in the FID to the number actually required for spectral analysis at the chosen spectral width. Downsampling (also called decimation) is the final step in digital signal processing.

experiment — In VNMR, a directory in which parameters and data are stored.

FID — Free induction decay. Signal observed from an experiment.

Fourier transform Converts time-domain data (FID) into frequency domain (spectrum).

FRED software (Full Reduction of Entire Datasets) Optional software package available from Varian that analyzes data by more advanced mathematical methods than are traditional in NMR analysis. FRED extracts carbon-connectivity information from data from INADEQUATE experiments.

***GEMINI 2000* system** Type of Varian NMR spectrometer system.

GLIDE A VNMR user interface

host computer Sun workstation that controls the spectrometer system.

IPA (interactive parameter adjustment) Window in which the values of up to five parameters can be changed by moving a horizontal slider with the mouse.

linear prediction Uses information from the "center" of the FID to extend the FID either in a reverse direction (to improve early point in the FID) or in a forward direction (to eliminate truncation problems). Following this process, the FID is then Fourier transformed in the usual way.e

lock Circuitry that compensates for long-term changes in the superconducting magnet field.

macro Single command that duplicates any series of commands, macros, and parameters enterable on the keyboard

MAGICAL MAGnetic Instrument Control and Analysis Language. Macro language built into VNMR

MERCURY Type of Varian NMR spectrometer system.

MERCURY-VX *MERCURY* with upgraded acquisition computer running VxWorks™.

NMR system administrator Special user, with name `vnmr1`, who is the only user with permission to change files found in the top VNMR system directory. `vnmr1` is also a regular user of VNMR, with permission to run NMR experiments, process data, etc.

NMR system console Main unit of NMR spectrometer, housed in one to four cabinets.

OpenWindows UNIX windowing environment.

oversampling Acquiring data with larger spectral width using a larger number of data points, as compared to acquisition without digital signal processing (DSP). Oversampling the data is the first step in performing DSP.

Performa modules Optional pulsed field gradient (PFG) modules for high-resolution liquids experiments.

remote status module Small case containing indicators and displays that show status and temperature or the variable temperature unit, lock level, acquisition, and other information about each active rf channel

root Top-level directory of a UNIX file system. Also, login name of the UNIX system administrator.

shims Set of coils inside the magnet that induce changes in the shape of the magnetic field.

Solaris Sun Microsystems operating environment. Includes SunOS.

STARS software Optional software available from Varian that simulates single-pulse experiments on solids under magic-angle spinning (MAS) or VAS conditions.

SunOS Sun Microsystems operating system. Part of the Solaris.

UNITY system Type of Varian NMR spectrometer system.

UNITY*INOVA* system Type of Varian NMR spectrometer system

UNITY*plus* system Type of Varian NMR spectrometer system.

UNITY-series systems UNITY*INOVA*, UNITY*plus*, and UNITY spectrometer systems.

user library User-contributed files placed in the `userlib` directory.

VNMR Name of Varian's NMR application software package.

vnmr1 Login name of the NMR system administrator.

VnmrI Version of VNMR for IBM workstations.

VnmrSGI Version of VNMR for SGI workstations.

VXR-S Type of Varian NMR spectrometer system.

VXR-style systems Gemini, VXR-4000, and XL spectrometer systems.

workspace VNMR display screen background where no windows appear.

Symbols

-#+ button, 42
'...' (single quotation marks) notation, 95
+Abort Acq button, 207
.bru files, 290
.def files, 278
.fid files, 279, 282
.login file, 48
.macdir for GLIDE experiments, 55
.par files, 278, 279
/ (slash symbol) directory, 34
->AV button, 72, 74
->PH button, 72, 74
? (question mark) notation, 96
\ (backslash) notation, 94, 197

Numerics

10-Gauss Warning Sign, 18
1D Data Display menu, 77
1D Data Display Secondary menu, 78
1D Data Manipulation menu, 77
1D Data Processing menu, 71
1D Display Size Selection menu, 78
1D experiment, customizing, 55
1D Plotting menu, 78
1D Processing Parameter Setup menu, 72
1D Pulse Sequence Setup menu, 68
1D Pulse Sequence Setup Secondary menu, 69
20-bit digitizer, 215
2D button, 69
2D Data Display menu, 79
2D Data Display Secondary menu, 80
2D Data Manipulation menu, 79
2D Data Processing menu, 73
2D Display Size Selection menu, 79
2D Interferogram Processing menu, 74
2D Line List button, 82
2D Peak Picking Automatic menu, 75
2D Peak Picking Edit menu, 76
2D Peak Picking File menu, 76
2D Plotting menu, 80
2D Processing Parameter Setup menu, 74
5-Gauss Warning Sign, 17, 19
60-dB fine attenuator, 193
6-dB fine attenuator, 193
90-degree pulse length, 114, 188

A

A2B button, 83
A2B2C button, 84
A2BC button, 84
A2BCD button, 84
A3B button, 84
A3B2 button, 84
A3B2C button, 84
A3BC button, 84
aa command, 203, 207
AB button, 83
ABC button, 83
ABCD button, 84
ABCDE button, 84
Abort Acq button, 65, 203
abort acquisition, 203
abort experiment in progress, 65
absolute cursor position, 247
absolute location, 272
absolute pathname, 37
absolute-intensity mode, 232, 245
absolute-value 2D experiments, 222
absolute-value mode, 72, 74, 79, 80, 225
absorption spectrum, 224
Acetone button, 68
acqbin directory, 34
acqfil directory, 208
Acqi button, 66
acqi command, 40, 148, 154, 207
acqi('par') command, 156, 159
Acqproc command (UNIX), 208
Acqstat command (UNIX), 207, 208
acqstat macro, 40
acqstatus parameter, 208
Acquire button, 66, 67, 148, 198
Acquire menu, 70
acquiring data, 183
acquisition, 198–209
  aborting, 203
  activity log, 208
  automated, 98
  automatic lock initiation, 133
  codes, 208
  data station restrictions, 148
  done code, 208
  error, 204
  error code, 208
  information, 208
  initiating, 198
  log, 278
  multiple users, 207
  processes, 24
  queueing, 30, 200
  remote control, 207
  resume after stopping, 202
  stopping, 202
  stopping early, 202
  time, 140
  time estimate, 189
  time too short, 227
  windows, 49
acquisition commands directory, 34
acquisition computer, 24, 203
Acquisition Controller board, 24
acquisition log file, 37
Acquisition Status window, 28, 40, 41, 44, 49
Acquisition window, 28, 31, 40, 41, 42, 44, 49, 148, 149
acrobat directory, 34
adaptive acquisition, 33
ADC bits displayed, 155
ADC overflow, 215
add button, 83
Add Spectrum button, 82
add spectrum into add/subtract experiment, 82
Add/Sub button, 81, 86
Add/Subtract menu, 82
addi command, 83

additive weighting constant, 72, 221, 223
addpar macro, 111, 228, 236
address of local Ethernet node, 283
Adj IS button, 77
Adj VS button, 77
Adj Weighting button, 71, 73, 74
Adj WP button, 77
Adjust button, 75
adjust integral height, 253
adjust integral scale, 77
adjust vertical scale, 77
adjust width of plot, 77
advanced operating features, 29
aexppl macro, 250
ai command, 232, 245
aig parameter, 245
alfa parameter, 187, 188, 216
algorithm, autophase, 225
All Contours button, 80
All Params button, 78, 80
allzs method, 145
alock parameter, 132, 133, 154
AM (Bruker) data, 289
AMX (Bruker) data, 289
analog anti-aliasing filter, 210
analog-to-digital converter (ADC), 24, 209
Analyze button, 66, 80
Analyze menu, 81
angled brackets (< or >) notation, 21
ap command, 261
aph algorithm, 225
aph command, 225
aph0 algorithm, 225
aph0 command, 225
aphb command, 225
apinterface parameter, 192
app-defaults directory, 45
append text to current experiment text file, 197
Applications Mode menu, 70
appmode parameter, 70
APT button, 68
apt macro, 32
arguments to commands, 93
array index, 95
array macro, 95
arraydim parameter, 200
arrayed experiment dimension, 200
arrayed experiments, 278
arrayed parameters, 95
arraying a parameter, 31, 32
assign button, 85
assign macro, 85
asynchronous decoupler mode, 190
at parameter, 140, 187
atext command, 197
Attached Proton Test, 68
ATTEN pushbuttons, 116
ATTEN readout, 115
attenuator configurations, 191, 192
au command, 138, 198, 200, 201
audio filter, 187
auto assign button, 85
Auto button, 75
auto button, 140, 161
autolist macro, 201
Automake Shimmap button, 170
automated
  acquisition, 98
  data acquisition, 98
  plotting, 99
  processing, 99
  shimming, 172
Automated Shimming menu, 178, 181
automatic
  block-size processing, 204
  phase calculation, 77
  phasing, 225
  selection of peak regions, 77
  shimming, 36, 130, 139, 142, 144, 145, 161
Automatic button, 71, 198
Automatic COSY Analysis menu, 82
Automatic DEPT Analysis menu, 81
automatic gain, 205
automatic lock
  full optimization, 134
  optimizing Autolock, 133
  simple Autolock, 132
automatic phasing algorithms, 225
automatic teller machine (ATM) cards caution, 19
autoname command, 278
Autophase button, 77
AUTOSHIM menu, 162
autoshim method, 158
Autoshim on Z button, 172
Autoshim, see automatic shimming
autostack macro, 99
AV button, 80
av command, 225
awc button, 72, 223
awc parameter, 221
AX button, 84
AX2 button, 84
AX2Y button, 84
AX3 button, 84
axes, positioning, 262
axis parameter, 232, 246, 249, 253
axisf parameter, 232, 234
AXY button, 84
AXYZ button, 84

B

B shimming criterion, 140
background Autoshim, 139, 145
background mode operation, 30
Backup File button, 76
bad shimming criterion, 140
bandpass filter, 212, 217
bandwidth of digital filter, 212, 217
bar command (UNIX), 291
baseline correction, 77, 242, 252
baseline flatness, 188
baseline performance, 214
Bayes software package, 33
BC button, 77
bc command, 252
bearing air, 105
beginning acquisition, 70

Benzene button, 68
best button (acqi), 156
beta parameter, 187
bin directory, 34
BINOM button, 69
binomial water suppression, 69
blanked amplifiers, 188
block-size storage, 203
borders, showing and hiding, 263
Both button, 75
Box button, 71, 73, 74, 75, 76, 83, 234, 239, 243
box command, 273
bpa macro, 261
Brickwall filter, 214
broadband switchable probe, 23
Broaden button, 72
Bruker data processing, 227
Bruker data, autophasing, 225
Bruker tape, 290
bs parameter, 156, 158, 203
btune macro, 124, 125
buttons on menus, 59
By Date button, 89
By Size button, 89

C

C13 button, 68
c13 parameter set, 145
C13, CDCl3 button, 67
calcdim command, 200
calculate
    contour plot, 80
    synthetic spectrum, 85
calculating
    field maps, 170
calfa macro, 216
calibration
    automated, 98
Cancel button, 75
Cancel Cmd button, 65
cancel correction, 252
cancel currently active command, 65
cancel integral reset points, 253
carbon connectivities, 33
carbon spectrum plot, 250
carbon-carbon connectivity 2D, 70
cat command, 277
cautions defined, 17
cd command (UNIX), 37
cd command (VNMR), 275
cdc command, 252
$CDCl_3$ as solvent, 67
CDCl3 button, 68
CDE menu, 50
CD-ROM drive, 24
celem parameter, 200
Center button, 78, 79
center button of mouse, 42
center command, 250
center of the screen/page, 78, 79
centersw macro, 185
chained experiments, 201
CHAN switch, 115
change
    directory, 37, 275
    filename, 276
change bar, 22
Change button, 88
change macro, 106
channel selection, 25
channels, rf, 24
chart parameters, 232
chemical shift scale, 79
chemist-style parameters, 261
clear
    add/subtract experiment, 82
    text file of current experiment, 197
    weighting parameters, 72, 74
Clear button, 76, 82
clicking a mouse button, 42
Clock program, 50
CLOSE button (acqi), 149, 150, 162
closed icons, 51
closing a window, 50
closing Plot Designer, 271
coarse shim controls, 163
coarse shim gradients, 136
coefficients for digital filtering, 210, 212
coefficients for filter computation, 217
color command, 257
color for graphics screen, 272
Color Map button, 74, 79
color printing, 257, 258
Color Selection window, 258
combination experiments
    customizing, 56
    processing and plotting, 57
Combine button, 76
command line editing, 97
command mode, 93
commands
    arguments, 93, 94
    defined, 93
    entry, 94
    help files, 34
    interactive, 94
    interspersed with parameters, 94
    names, 93
    sequential execution, 94
    types, 93
Comment button, 76
compare shim values in files, 138
compiled sequences library, 36
completed transients, 188
complex data point, 227
compress command (UNIX), 292
compress double-precision FID data, 293
compress FID files, 292, 293
compressfid command, 293
computed data, 281
computer
    acquisition, 24
    host, 23, 25
    Host-Acquisition Link, 24
config macro, 92, 193
Configuration menu, 92
configuration parameter file, 36

Configure button, 91
configuring hardware, 92
Connect button (acqi), 150
CONNECTED message, 49
conpar file, 36
console, 23
CONSOLE shell window, 48
construct a shim method, 142
CONT message, 45
CONTENTS file, 38
continuous wave (CW) modulation, 191
Contour button, 79
contour plot, 45, 80
control temperature, 196
Control-d key combination, 91
Control-h key combination, 97
Control-n key combination, 97
Control-p key combination, 97
Control-U key combination, 97
conventions used in manual, 21
convert
    Bruker data, 289
    data between systems, 286
    multiple FID element into a single FID, 229
    VXR-style FID file to VNMR, 288
convert command, 287, 288
convertbru command, 227, 289, 290
Copy button, 91
copy command, 276
copying
    directories, 276
    files, 91, 276
correct saved parameter sets, 280
cosine transform, 224
COSY analysis, 82
COSY button, 69, 81
COSY correlation map, 80
cosy macro, 32
COSY with double-quantum filter, 70
COSYPS button, 69
coupled spectra with NOE, 190
cp command, 277, 282
cpos_cvt command, 287
cr parameter, 184, 185, 239
create
    directory, 276
    linear prediction parameters, 228
    new directory, 88
    new experiment, 67
Create New button, 67, 88
credit cards caution, 19
crf parameter, 234
criterion for shimming, 141
criterion values for Autoshim, 140
crl command, 248
cross-polarization pulse sequence, 69
CT message, 49
ct parameter, 96, 188, 202
ctext command, 197
ctune macro, 124, 126
curexp parameter, 277
current directory, 87, 88
current experiment number, 45
current plane, 45
current working directory, 275
currently active experiment, 277
cursor, 41
Cursor button, 71, 73, 74, 75, 76, 83, 234, 239, 243
cursor movement, 234
cursor position, 184
cursors, 27, 59
customizing experiments, 55
customizing the menu system, 64
cutoff parameter, 245
cutoff steepness, 214
cz command, 241, 253

D

d suffix, 95
d1 parameter, 187, 188
d2 parameter, 187
D2O button, 68
D2PUL button, 69
data analysis tools, 81
Data button, 87
data compression, 292
data directory, 37
data files format, 287
data processing methods, 227
data recall
    in CDE, 58
    using VNMR menus, 58
data station and acquisition, 148
data storage files location, 37
data storage for experiments, 31
date of acquisition, 200
date parameter, 200
DC button, 77
dc command, 252
dc level, 223
DC(f1) button, 80
DC(f2) button, 79
dcg parameter, 252
dcrmv parameter, 223
dd command, 289
dd command (UNIX), 290
decaying exponential function, 221
decimation, 210
decomp command, 287, 288
deconvolution, 222
Deconvolution button, 81
Deconvolution menu, 85
deconvolution starting point, 85
decoupled spectrum without NOE, 190
decoupler
    array of offset values, 185
    attenuation, 193
    field strength, 193
    fine power level, 193
    frequency, 95
    high-power caution, 193
    homonuclear control, 191
    mode, 190
    modulation, 193
    modulation mode, 194
    offset, 185

power, 193
power level, 193
programmable, 194
sequence, 194
status, 190
time-sharing, 191
waveform generator, 194
decoupler coil caution, 125
def_osfilt parameter, 214
Default button, 88
default directory, 275
default value of parameter, 96
defaultdir parameter, 88, 275
delay period, 187
delete
experiment file, 67
files and directories, 87
Delete button, 67, 87
delete command, 276
Delete key, 97
delta parameter, 185, 239
deltaf parameter, 234
DEPT analysis, 81
DEPT button, 68, 81
DEPT pulse sequence, 68
dept.out file, 82
depth indicator, 102
detuning of the probe, 114
deuterated lock solvent, 130
deuterated solvents, 101
deuterium decoupler channel, 192
deuterium frequency, 184
deuterium gradient shimming, 168
deuterium rf, 24
devicenames file, 36
devices defined as active, 92
devicetable file, 271
df command, 71, 231, 232, 234
dfid command, 233
dfrq parameter, 152, 183
dfrq2 parameter, 183
dfrq3 parameter, 183
dfrq4 parameter, 183
dfsa command, 237
dfsan command, 237
dfsh command, 237
dfshn command, 237
dfsn command, 237
dfww command, 237
dg command, 47, 112
dg parameter, 112, 189
dg program, 44, 47
dg1 macro, 112
dg1 parameter, 112
dg2 macro, 112
dg2 parameter, 112
dglp command, 112, 228
dgs macro, 112, 127, 136
dgs parameter, 112
dhp parameter, 193
diagnostic messages, 48
diffshims macro, 138
diffusion software, 33
digfilt macro, 218
Digital Acquisition Controller board, 24
digital filter, 209
digital filtering, 228
digital integral amplitudes, 254
digital quadrature detection, 218
digital resolution, 140, 247
digital signal processing (DSP), 209
digitization errors, 209
dimension of an experiment, 200
dir command, 276
directories, 34
change, 88
create new directory, 276
delete, 87
file suffix on Ethernet, 284
make copies, 276
remove, 276
rename, 276
size of entries, 89
sort entries, 89
transfer over Ethernet, 282
user, 36
working, 37
Directory button, 89
Directory menu, 88
Directory Secondary menu, 88
dispersion spectrum, 224
display
1D spectrum and scale, 77
2D contour display, 79
2D interferogram as contour map, 74
ADC bits, 155
arrayed parameter value, 96
box drawing, 273
data stacked and whitewashed, 80
Ethernet nodes available, 282
Ethernet remote nodes, 282
experiment log file, 207
experimental spectrum, 83
FID, 154, 231
FID last acquired, 155
FIDs horizontally, 237
file contents, 277
files, 46, 90
fit a line to data points, 86
full spectrum, 250
gray scale image, 79
grid lines, 155
inset of spectrum, 242
integral intensities, 78
integral reset points, 253
integrals, 250
iterative optimization spectrum, 85
last fit results, 85
library of experiment files, 67
line drawings, 272
linear prediction parameters, 228
listing of last spin simulation, 84
local Ethernet node, 283
modes, 232
numerical integral amplitudes, 254
one or two cursors, 231
output devices, 92
parameter groups, 112

parameter value, 96
peak frequencies, 246
plot jobs in queue, 255
pulse sequence as a graph, 189
pulse sequences, 188
regression analysis results, 87
remote directory on Ethernet, 283
scale under spectrum or FID, 246
second cursor, 234
shim gradient parameters, 136
simulated spectrum, 85
spectra, 243
spectra horizontally, 78
spectral line frequencies and amplitudes, 78
spectrum, 159, 225, 231
spin simulation parameters, 83
summed FID, 155
synthetic spectrum, 85
text file in current experiment, 197
time for experiment, 70
vertical scale, 232
whitewashed FIDs, 237
Display button, 66, 75, 81, 90
display button, 85
display command, 253
Display FID button, 71
display monitor, 44
display parameter set, 243
display screen, 27
Display Shimmap button, 170
divide spectrum into regions with peaks, 253
dla macro, 85
dli command, 253
dll command, 246
dlni command, 253
dlp parameter, 193
dm parameter, 190, 194, 195
dm2 parameter, 191
dm3 parameter, 191
dm4 parameter, 191
dmf parameter, 193, 194, 195
dmf2 parameter, 193
dmf2adj macro, 194
dmf3 parameter, 193
dmf3adj macro, 194
dmf4 parameter, 193
dmf4adj macro, 194
dmfadj macro, 194
dmg parameter, 72, 74, 79, 80
dmgf parameter, 156
dmm parameter, 191, 194, 195
dmm2 parameter, 193, 194
dmm3 parameter, 193, 194
dmm4 parameter, 193, 194
DMSO button, 68
dn parameter, 185
dn2 parameter, 185
dn3 parameter, 185
dnode command, 282, 285
dof parameter, 152, 185
dof2 parameter, 185
dof3 parameter, 185
done codes, 208
DOS file system, 291
double-backslash character, 197
double-precision VNMR FID data, 293
double-quantum filtered COSY, 70
down button, 155
down-arrow key, 97
downsamp parameter, 217
downsampling data, 210
downsampling factor, 217
dp output, 87
dp parameter, 216, 293
dp-cubic button, 87
dp-exp button, 86, 87
dpf command, 246
dpir command, 254
dpirn command, 254
dp-linear button, 86
dp-quad button, 86, 87
dps command, 189
dpwr parameter, 193, 194, 195
dpwr2 parameter, 193
dpwr3 parameter, 193
dpwr4 parameter, 193
dpwrf parameter, 193
dpwrf2 parameter, 193
dpwrf3 parameter, 193
dpwrm parameter, 193
dpwrm2 parameter, 193
dpwrm3 parameter, 193
DQCOSY button, 70
DraftMaster plotter, 255
DraftPro plotter, 255
draw box, 273
draw command, 272
draw line, 272
dres command, 247
dres parameter, 194
dres2 parameter, 194
dres3 parameter, 194
dres4 parameter, 194
drift correct 2D data set, 79
drift correct spectrum, 77
ds button, 243
ds command, 73, 225, 231, 232, 237, 242, 253
Dscale button, 71, 73, 234, 239
dscale command, 246
dscoef parameter, 217
dseq parameter, 194
dseq2 parameter, 194
dseq3 parameter, 194
dsfb parameter, 217
dshim macro, 139
dslsfrq parameter, 217
DSP (digital signal processing), 209
compressing DSP FID files, 293
dsp parameter, 211
Dssa button, 78
Dssh button, 78
dtune macro, 124
dwell time, 185

E

e macro, 104
E shimming criterion, 140

eaddr command, 283, 285
Edit button, 75, 82, 91
edit macro, 197
edit text files, 91, 197
efficient mode decoupling, 194
Eject button, 55
eject button (acqi), 150
Eject button (GLIDE), 104
eject command (UNIX), 291
ejecting a sample, 104, 150
elist command, 283
English-language parameter format, 78, 261
enlarge graphics window, 47
enter program, 55
entering commands, 94
entering VNMR, 39
enumerated characters, 96
enumerated string values, 96
eread command, 282, 284, 285
ernst command, 188
errlog command, 45, 209
errloglen parameter, 45, 209
error codes, 208
error handling control, 134
error messages display, 45
error messages on limNET, 285
Ethernet communication, 24
Ethernet network, 281
ethers file, 285
ewrite command, 283, 284, 285
excellent shimming criterion, 140
exit command, 41
Exit VNMR button, 46, 91
exiting VNMR, 40, 51, 91
Exp # button, 67
exp# file name, 277
exp1 through exp9 experiments, 31, 67
exp5 experiment, 82
expactive command, 208
Expand button, 71, 73, 74, 75, 76, 83, 234, 239, 243
experiment
  abort, 65
  active, 200
  completed FIDs, 200
  dimension, 200
  files, 67
  lock mode, 206
  lock system, 206
  locked, 207
  log file, 207
  number, 45
  stop acquisition, 202
  text files, 197
Experiment button, 54
experiment time, 189
experiments
  accessing GLIDE, 55
  customizing using GLIDE, 55
  data collection, 277
  data storage, 31
  defined, 31, 277
  display experiment list, 31
  files, 277
  introduction of computed data, 281
  multiFID, 31
  multiple, 32
  number, 31
  path to experiment, 277
  repeating, 106
  run unlocked, 132
  running standard, 54
explib command, 31, 32
explicit acquisition compatibility, 215
explog command, 207
exponential analysis plot, 81
Exponential button, 81
exponential least-squares analysis, 81
exponential weighting, 72, 221, 223
export directory, 34, 36
exptime command, 189
extract files from VXR library, 287
extract shim parameter values, 138

F

f command, 250
F1 Mode button, 80
F1 Transform button, 74
F19 button, 68
F1–F9 keys, 43
F2 Mode button, 80
fb parameter, 187
fdformat command (UNIX), 291–292
FID
  display, 154, 231, 236
  display parameters, 232
  files, 37
  library, 34
  phase rotation, 233
  plotting, 236
  raw data file, 37
  shimming on the, 142
  start of plot, 232
  storage, 31, 37
  updating, 234
  vertical display position, 232
  vertical scale adjustment, 234
  viewing a particular FID, 233
  windowing mode, 234, 235
FID button (acqi), 149, 154, 155
FID Display Menu, 234
fid file, 37, 278
FID output from real-time DSP, 216
fidlib directory, 34
fidpar macro, 236
FIDs
  acquisition time too short, 227
  completed in experiment, 200
  composite displays, 237
  compressing FID data files, 292
  compute FID file, 281
  convert multiple FID into single FID, 229
  dc level, 223
  distortion from hardware, 227
  extend direction, 227, 296
  intensity, 223
  left shifting, 226

noise level, 209
phase rotation, 226
retrieve FIDs in FID file, 279
saving, 277
stopping spike at start of FID, 188
weighting function, 221
write FID data text file, 278
field homogeneity quality, 139
field offset, 136
field offset control, 184
fifth rf channel parameters, 110
File button, 46, 66, 75
File Info button, 87
file parameter, 109
files
compressing, 292
creation, 276
delete, 87, 276
display contents, 277
Ethernet filename suffixes, 283
experiments, 67
make copies, 276
overview of structure, 35
rename, 276
security maintenance, 284
sharing using a floppy, 291
transfer over Ethernet, 282
files command, 90
Files Data
menu, 90
Secondary menu, 90
Files Information menu, 89
Files Main menu, 87
Files Secondary menu, 90
files system, 34
Files Tape menu, 89
filter cutoff, 210
filter non-linearities, 227
filtering algorithm, 209
filtfile parameter, 213, 218
filtlib directory, 213, 218
Find Correlations button, 82
fine attenuator, 193
fine power control, 191
fine shim gradients, 136
finite impulse response (FIR) file, 213, 218
first button (acqi), 156
first-order baseline correction, 242, 252
fit a line to data points, 86
Fit button, 85
fit current spectrum, 85
fit line to data points, 86
five-spin system, 84
fixpar macros, 109
flag parameters, 96
flammable gases warning, 18
Flip button, 47, 65
flip command, 47
flip time, 188
floppy disk drive, 291
fn parameter, 223, 253
FN Small button, 72, 74
Fold buttons, 80
format of text files, 286
Fourier number, 72, 74, 95
Fourier transformation, 221, 223
complex, 227
data processing, 227
in progress, 45
number of points, 223
output data, 224
real, 227
spectra, 71
four-spin system, 84
fourth rf channel parameters, 110
fr macro, 243
FRED software package, 33
free induction decay. See FIDs
free-form arguments, 94
frequency referencing, 247
frequency shift of spectral data, 227
frequency-dependent phase shift, 216
frequency-shifted quadrature detection, 218
fsq parameter, 218
ft command, 221, 223, 227
FT message, 45
ftp command, 282
Full Analysis button, 82
Full button, 71, 73, 74, 76, 83, 234, 239, 243
full command, 250
full display of plot image, 250
Full Integral button, 73
full optimization of lock, 134
Full Screen button, 78, 79
full screen/page, 78, 79
full set of transforms, 73
Full Transform button, 73
Full with Traces button, 79
fully automatic Autoshim, 139
function key actions, 231
function keys, 43
function keys to select menu choice, 59
fuzzy logic, 225

G

ga command, 138, 198, 200, 204
gain from real-time DSP, 215
gain parameter, 154, 206
GARP decoupling, 194
Gaussian apodization, 222
Gaussian line shapes, 222
gaussian macro, 222
Gaussian time constant, 72, 221, 223
Gaussian time constant shift, 72, 223
GEMINI 2000
decoupling values, 195
probe tuning, 124
Gemini systems, 281
generating pulse sequences, 91
generic plotting macros, 250
gettxt command, 197
gf button, 72, 223
gf macro, 154, 156, 159
gf parameter, 221, 222
gfs button, 72, 223
gfs parameter, 221
GLIDE

button, 49, 53, 54, 65
command, 49, 53
directory, 34
files, 34
opening and closing, 53
user interface, 28, 49
global file, 37
gmapshim macro, 172, 176
gmapsys macro, 170, 172, 177
Go button, 70, 198
Go button (GLIDE), 55
go command, 32, 115, 138, 183, 198, 200, 203, 207
go('acqi') command, 156
Go, Periodic Wft button, 71, 204
Go, Wft button, 70, 198
go_ macro, 198
gotolink cpr_j
jplotscale, 269
gotolink cpr_r
rtcmx, 279
Gradient Autoshim on Z button, 176
gradient autoshimming, 168
Gradient Autoshimming Files menu, 172, 178, 181
Gradient Nucleus Parameter Setup menu, 177
Gradient Shim Setting menu, 178, 180
Gradient Shimming Display menu, 178, 180
Gradient Shimming Files menu, 178, 179
Gradient Shimming Map menu, 178, 179
Gradient Shimming Plot menu, 178, 180
Gradient Shimming Setup menu, 177, 178, 179
Gradient Shimming System menu, 170, 177, 178
gradient systems, 24
gradient to be shimmed, 141
gradtype parameter, 196
graphical probe tuning, 116
graphics screen line drawing capability, 272
graphics window, 44, 46
covering text window, 65
enlarge, 66
grayscale image, 79, 80
Grid button (acqi), 155
grid lines, 155
Grid Off button (aqi), 155
grid, magnetizing and demagnetizing, 263
grid, showing and hiding, 263
gshimlib directory, 172
gzip command (UNIX), 293
gzsize parameter, 177
gzwin parameter, 170

H

H1 button, 68
h1 parameter set, 145
H1,CDCl3 button, 67
H2 button, 68
halt command, 203
hard disk drive, 23
Hardware button, 92
hardware caused distortions, 227
hardware configuration, 92
hardware simple Autolock, 132
hardware Z1 Autoshim, 139
Hd All button, 77
Hd Box button, 76
Hd Lbl button, 77
Hd Pk button, 76
HdNum button, 76
hdwshim parameter, 139, 145
hdwshiminit parameter, 145
hdwshimlist parameter, 145
heat-exchange bucket, 196
helium contact with body, 18
helium gas flowmeters caution, 20
Help button (menu system), 59, 65
help directory, 34, 70
help files customization, 64
Help screen, 59, 65
HET2DJ button, 70
HETCOR button, 69
heteronuclear correlation, 69
heteronuclear decoupling, 194, 195
heteronuclear J-resolved 2D, 70
Hewlett-Packard plotters, 78, 255
Hewlett-Packard printers, 255
Hewlett-Packard raster mode, 255
hexadecimal codes for shim group, 143
high rf band, 184
high-power amplifiers cautions, 20
high-resolution plotter mode, 257
high-speed line control, 24
ho parameter, 237
HOM2DJ button, 70
Home button, 88
home directory, 34, 36, 37, 88
homo parameter, 191, 194
homo2 parameter, 192
homo3 parameter, 192
homo4 parameter, 192
homogeneity adjustments, 135–139
homogeneity quality, 139
homonuclear correlation, 69
homonuclear decoupling, 194, 195
homonuclear decoupling control, 191
homonuclear J-resolved 2D, 70
homonuclear operation, 185
homospoil gradient shimming, 174
homospoil process, 206
homospoil status, 190
horizontal axis selection, 80
host computer, 25, 203
Host-Acquisition Link (HAL), 24
hosts file, 282, 285
hoult macro, 188, 216
HP 7475A plotter, 255
HP 7550A plotter, 255
HP Params button, 78
hpa command, 262
HPGL graphics language, 255
Hproj (max) button, 75
Hproj (sum) button, 75
hs parameter, 206
hst parameter, 206
htune macro, 124, 126
Hz to plotter units, 273
hzmm parameter, 250
hztomm command, 273

Index

I

I2 field, 284
IBM RS/6000 computer, 290
IBM workstations, 25
icon for closed window, 28, 50
idelay statement, 159
ilfid command, 229
Image button, 79, 80
Imaginary button, 71, 234
imaginary channel, 224, 234
Imaging button, 70
imaging probe tuning, 116
Improving Results
    suggestions, 176
in parameter, 128, 134
in vivo spectra phasing, 225
INADEQUATE pulse sequence, 70
INADQT button, 70
increment FID/interferogram index, 72, 223
indefinite acquisition, 188
INEPT button, 68
INEPT pulse sequence, 68
Info button, 76
initiate acquisition, 198
inline DSP, 210, 211, 218
input window, 44, 45
ins parameter, 252, 253
insert button (acqi), 150
Insert button (GLIDE), 55, 105
inserting a sample, 105
inset command, 242
inssref parameter, 253
insufficient free disk space, 198
integer arguments, 94
integral blanking mode, 254
integral intensities, 78
integral offset, 232, 242
integral position with respect to spectrum, 232
integral reset mode, 239, 241
integral reset points, 77, 253
integral scale, 242
integral scale adjustment, 77
integral value scaling, 253
Integrals button, 78
interactive
    adjust 1D spectrum, 77
    adjust 2D contour display, 79
    adjust gray scale image, 79
    adjust stacked and whitewashed data, 80
    Autoshim, 139
    Autoshim mode, 144
    commands, 94
    define shim methods, 143
    FID manipulation, 233
    FID windowing mode, 234, 235
    files program, 275
    integral reset mode., 239, 241
    lock display, 151
    parameter adjustment, 159
    phasing mode, 234, 235, 240
    probe tuning, 116
    spectra display, 237
    spectral windowing mode, 239, 240
    spectrum display, 225
    weighting, 223
    zero and first order baseline correction mode, 241
Interactive 1D Spectrum Display Menu, 238, 239
Interactive 1D Spectrum Display menu, 73
Interactive 2D Color Map Display Main menu, 74
Interactive 2D Display Projection menu, 75
Interactive 2D Peak Picking Main menu, 75
interactive acquisition window, 148–162
Interactive Add/Subtract menu, 83
Interactive button, 77
interactive display programs, 231
Interactive Mode button, 82
interactive programs with menus, 60
Interactive Weighting menu, 71, 72
interface board, 192
interleaving FIDs, 229
interlock parameter, 128
intermodulation distortions, 205
Internet Protocol (IP), 281
intmod parameter, 78, 249, 252
inverted lines spectra, 225
io parameter, 232, 240, 242
ionic samples, 114
IP (Internet Protocol), 281
IPA (interactive parameter adjustment), 159
IPA button, 159
ipulse statement, 159, 160
is parameter, 239, 242, 253
isadj macro, 253
iterate button, 85
iterative optimization, 85

J

jdesign macro, 264
jexp command, 32, 207
join an experiment, 32
join experiment, 67
jplot command, 262, 264
J-resolved 2D, 70, 80

K

k suffix, 95
K symbol, 223
kermit directory, 34
kermit program, 34
kermit.doc file, 34
keyboard, 27, 42
keyboard entry of macros, 33
kill command (UNIX), 208, 286
killplot macro, 255

L

L shimming criterion, 140
L1 to L10 keys, 43
L7 function key, 50
Label button, 76
Laboratory Information Management Network, 281
landscape view, plot configuration, 270
Large button, 72, 74

LARGE button (acqi), 149
large command, 47
large graphics window, 46
large transform with zero filling, 72, 74
LaserJet Plus printer, 255
lb button, 72, 223
lb parameter, 221, 222
Left button, 78, 79
left button of mouse, 42, 59
left command, 250
left half of the screen/page, 78, 79
left phase, 224
left-arrow key, 97
left-shifting a FID, 226
length of 90-degree pulse, 188
lf command, 108, 276
lfs (low-frequency suppression), 228
liamp parameter, 253
lib directory, 34
libraries of software, 34
Library button, 67
lifrq parameter, 253
limNET protocol, 281
limNET server shutdown, 286
limnetd process, 286
line broadening, 221
line broadening parameters, 72
line broadening weighting, 72, 223
line listing on the current spectrum, 85
linear amplifier power control, 190
linear baseline correction, 252
linear modulators, 193
linear prediction
    algorithm, 228
    data processing method, 227
linear pulse amplifier, 24
linear x-axis scale, 86
linear y-axis scale, 86
line-drawing capability, 272
Lines button, 78
liquid column length, 101
list button, 84
list files, 276
listenon macro, 109, 138, 280
lkof parameter, 152
ll button, 85
llamp parameter, 246
llfrq parameter, 246
load
    parameter set into current experiment, 87
    parameters and data, 90
    shims, 90
    streaming tape to current directory, 89
    Varian data to current experiment, 87
Load button, 87, 90
load parameter, 136, 137, 154
Load Params button, 90
Load Shims button, 90
loc parameter, 106
local oscillator, 191
lock, 129–135
    effect of solvent, 130
    frequency, 24, 184
    gain, 131
    lock transmitter, 184
    mode, 206
    parameters, 130, 132, 152
    power, 131
    power and gain optimization, 133
    power when shimming, 139
    saturation, 139
    shimming on the, 142
    solvents, 110
    status, 151
    time constant control, 135
LOCK button (acqi), 149, 151
lock command, 134
LOCK display, 151, 153
lock frequency, 248
lock frequency acquisition window, 134
lock frequency, set, 153
lock level display, 43
lock level interlock, 134
LOCK menu, 151
lock receiver gain, 157
lock_N.primary file, 206
lock_N.secondary file, 206
lockacqtc parameter, 135
locked experiment, 207
lockfreq parameter, 152, 183, 184, 248
lockgain parameter, 130, 150, 152, 154
lockphase parameter, 152, 154
lockpower parameter, 130, 150, 152, 154
locktc parameter, 135
log file, 37, 208, 278
logarithmic x-axis scale, 86
logarithmic y-axis scale, 86
login command (UNIX), 40
login directory, 88
login macro, 109, 280
login prompt, 40
logout command (UNIX), 41
loose shimming criterion, 140, 162
Lorentzian lineshapes, 222
low rf band, 184
low-frequency suppression, 228
lp parameter, 216, 224, 225, 241
ls command (VNMR), 276
lsfid parameter, 156, 223, 226, 233
lsfrq parameter, 227, 229
lvl parameter, 241, 252
Lvl/Tlt button, 73, 239, 241

M

M shimming criterion, 140
Macintosh computer, 291
maclib directory, 34, 70, 98
macros
    automation, 98
    defined, 32, 93
    keyboard execution, 33
    language, 32
    library directory, 34
    names, 32
MAGICAL II language, 32
MAGICAL II macro library, 34
magnet, 23, 25

magnet quench warning, 18
magnetic media caution, 19
magnetic tape operation, 289
magnetic tape unit, 23
magnetic tapes caution, 290
magnetization recovery to equilibrium, 188
Main Menu, 46
Main menu, 46, 60, 66
Main Menu button, 46, 65
main processor, 24
makefid command, 281
manual button, 161
manual directory, 34, 38
manual emulation shimming, 138
manual locking, 153
manual sample ejection and insertion, 103
Manual Shim menu, 156
manual shimming mode, 161
Mapping the shims, 169
Mark button, 76, 239
mark1d.out file, 85, 239
Massage button, 77, 79
MasterLog file, 208
mathematical expressions, 95
maximum transients accumulated, 202
maxpen parameter, 255, 256, 257
medium shimming criterion, 140, 162
medium-resolution plotter mode, 257
memory overflow from real-time DSP, 215
menu buttons, 46
menu command, 60
menu system, 44, 59
    customization, 64
    help files, 34
    interactive program menus, 60
    outline, 61, 62, 63, 64
    pulse sequence programming, 91
menulib directory, 34, 70
menus library, 34
metal objects warning, 17
method parameter, 139, 144, 145, 207
min button, 83
Minimum button, 82
minsw macro, 185
mkdir command, 276
MLEV-16 decoupling, 194
mnemonic parameter format, 78, 261
Mode label, 156
modifying the instrument, 18
More 1D button, 69
More button, 60, 66, 90
mount command (UNIX), 291
mouse arrow, 59
mouse button labels, 231
mouse buttons, 42
mouse device, 27, 41
move command, 272
move experiment to head of queue, 201
move to next command line, 97
movedssw macro, 217
moveossw macro, 213
movesw macro, 185
movetof macro, 184
mt command, 289
multi-FID experiments, 31
multiple data processing operations, 30
multiple data sets, 32
multitasking, 30
mv command, 276
mxconst parameter, 202

N

N15 button, 68
name of a macro, 32
nearest line, 246
needle micrometer, 25
network timeout, 285
network use of a tape, 291
new users, 59
newfs command (UNIX), 292
newshm macro, 143
next fid button, 72, 223
nitrogen contact with body, 18
nitrogen gas flowmeters caution, 20
nl command, 246, 247
nli command, 253
nm command, 232, 245
NMR spectrometer system units, 23
NMR system administrator, 36
NMR system console, 24
No Imag button, 71, 234
No Integral button, 73, 239
No WT button, 72, 74
nodes file, 282
NOE 2D correlation, 69
NOESY button, 69
noise command, 209
noise level of a FID, 209
noise limit, 246
noise reduction, 209
noislm macro, 246
non-linear baseline correction, 252
non-saturating lock power, 139
non-spin shims, 163
Normal button, 72, 74
normal size transform, 72, 74
Normalize button, 80
normalize vertical scale, 80
normalized display mode, 232, 245
notational conventions, 21
np parameter, 187, 223
nt parameter, 187, 188
nuclei selection, 110, 111
nucleus lookup files, 34
Nucleus Selection menu, 68, 110
nucleus standard parameter sets, 36
nucleus table, 183
Nucleus, Solvent button, 67
nuctables directory, 34
nuctabref file, 248
number of transients, 187, 188
numeric arguments, 94
numeric parameters, 94
numerical integral amplitudes, 254
numrfch parameter, 110

O

object preferences, setting, 265
observe button, 85
observe receiver gain, 157
opening a window, 51
OpenWindows windowing environment, 25, 33
optimizing Autolock, 133
optimum (“Ernst”) pulse width, 188
optimum lock parameters, 130
organic solvents, 114
Original button, 83
orthogonal data points, 227
oscoef parameter, 212
osfb parameter, 212
osfilt parameter, 214
oslsfrq parameter, 212, 218
Output board, 24
output devices, 92
oversamp parameter, 212, 214
oversampling amount, 214
oversampling data, 209
oversampling factor, 212, 213

P

p suffix, 95
p1 command, 188
p1 parameter, 187, 188
P31 button, 68
pacemaker warning, 17
pad parameter, 187
Page button, 78, 80
page command, 255
pages of plotter output, 254
panel menu, 159
panels of shims, 157
pap macro, 261
paramedit command, 112, 261
paramedit macro, 261
parameter sets, 107
    correct saved sets, 280
    filename storage, 110
    listing files, 108
    retrieval, 109
    standard parameter sets, 110
    storage, 36
parameters
    acquisition, 37
    adjusting and restoring plot, 269
    arrayed, 95
    baseline correction, 242
    chemist-style, 261
    common to experiments, 37
    create for current experiment, 111
    default values, 96
    defined, 93
    display groups, 112
    entering values by hand, 231
    entry, 95
    entry limitation, 96
    frequency-related, 183
    hardware autoshim, 145
    integer truncation, 96
    interactive parameter adjustment, 159
    line broadening, 72
    linear prediction, 228
    names, 94
    organization, 107
    phasing, 224
    plot list of values, 261
    Pulsed Field Gradient (PFG) module, 196
    resolution enhancement, 72
    retrieve from parameter file, 279
    rf channel related, 109
    selection, 72, 73
    shim gradients, 136
    turned off, 95
    types, 94
    update old parameter characteristics, 109
    value display, 96
    value ranges, 96
    weighting, 72
parameters, parameters, 262
Params button, 78, 80, 85
paramvi macro, 112
pards macro, 217
Parent button, 88
parent of a directory, 88
parentheses, 94
parfix macro, 280
parlib directory, 36, 107
parlp macro, 228
paros macro, 212
Part Integral button, 239
parversion parameter, 280
password prompt, 40
password selection, 40
pathname defined, 37
pathname to current experiment, 277
PC platform, 291
Peak button, 74, 75
peak frequencies, 246
peak regions selection, 77
Peaks button, 78
peak-to-peak noise, 246
pen and raster plotters, 258
pen command, 272
pen number, 272
pen plotters, 255
Performa PFG modules, 24
Performance Meter program, 50
Permanent menu, 46, 60, 65
pfgon parameter, 196
pfww command, 237
PH button, 79
ph command, 225
PH mode, 80
Phase button, 71, 73, 225, 234, 235, 239, 240
phase command, 225
Phase F2 button, 73
phase parameters, 225
phase rotation, 223, 226, 233
phase-sensitive COSY, 69
phase-sensitive mode, 72, 74, 79, 80, 225
phasing
    interactive, 235
    mode, 234, 240

spectra, 224
phasing parameter, 235, 240
phfid parameter, 156, 159, 223, 226, 233, 235
phosphorus spectrum plot, 250
pi3ssbsq macro, 222
pi4ssbsq macro, 222
pir command, 254
pirn command, 254
pl command, 249
plfid command, 237
plh macro, 249
pll command, 249
plot
axis below spectrum, 78
columnar line list, 249
currently displayed region, 249
customizing a, 263
editing with Region Editor, 266
exponential analysis spectra, 81
FIDs, 237
finish current plot and change paper, 78, 80
importing from VNMR graphics window, 265
integral with spectrum, 78
integrals, 250
parameters, 80, 232, 261
parameters on HP plotter, 78
peak frequencies, 249
peaks frequencies above peaks, 78
phosphorus spectrum, 250
proton spectrum, 249
pulse sequence, 188
pulse sequence as a graph, 189
scale under spectrum, 249
simulated spectrum, 86
spectrum, 78
start, 232
text file, 262
width, 232
Plot button, 74, 75, 77, 78, 79, 81, 82, 86, 87, 243
Plot Correlations button, 82
Plot Designer program, 262–271
plot macro, 250
plot menu file, 266
plot output, positioning, 262
plot parameters, adjusting and restoring, 269
plot, importing into a region, 266
plot1d macro, 250
plotter
attached to computer, 36
choices, 257
code, 255
color printing, 258
configuration, 255, 257
convert Hz or ppm, 273
draw box, 273
line drawing, 272
list of choices, 36
number of pens, 255
pen number, 272
plotter devices, 92
queue, 255
resolution, 256
selection, 257
size of plot area, 255
speed, 257
plotter parameter, 255
plotting
automated, 99
general rule, 232
plotting commands, 254
plp macro, 250
pltext command, 262
pltmod parameter, 249
points to Fourier transform, 223
pop-up menu, 150
portrait view, plot configuration, 270
Pos. Only button, 80
position plots and displays, 250
postacquisition DSP, 210, 217
Postscript devices, 262
PostScript output, 255
Postscript raster printers, 255
power mode, 225
ppa macro, 261
ppf command, 249
ppm scales calculation, 183
ppm to plotter units, 273
ppm units, 95
pps command, 189
preacquisition delay, 187
preamplifier saturation, 227
preparing samples, 101
preprinted chart paper, 262
previous command line, 97
primary lock, 206
print
all parameters, 261
exponential least-squares analysis, 81
gray scale image, 80
parameters, 78, 80, 261
text file, 271
working directory, 37
Print button, 81
printcap file, 271
printer
attached to computer, 36
devices, 92
list of choices, 36
printing, 271
color printing, 257
printoff command, 271
printon command, 271
Printout button, 82
probe, 23, 25
insertion, 113
protection, 198
removal, 112
ringing, 227
tune interface panel, 114
tuning, 25, 113–116
probe file macros, 113
probe file parameter, 113
probe_protection parameter, 198
proc parameter, 227
Process button, 66, 81
process data, 71, 99
process ID, 286
process number, 208

processed data storage, 31
procpar directory, 280
procpar file, 37, 278
programmable decoupling, 194
Proj button, 74
prosthetic parts warning, 17
proton gradient autoshimming, 168
proton spectrum plot, 249
ps command (UNIX), 286
pscale command, 249
Pseudo button, 74
pseudo-echo weighting, 74
pseudo-quadrature data, 227
psg directory, 36
psglib directory, 36
pslabel parameter, 45
ptext command, 271
public socket, 285
pulse breakthrough effects, 188
Pulse Sequence Controller board, 24
Pulse Sequence Entry Main menu, 91
pulse sequence implementation, 24
pulse sequence name, 185
pulse sequence programming, 91
pulse sequences
  graphical display, 188, 189
  library, 36
  plotting, 188
  requested by the operator, 45
  S2PUL, 185
  set up using a macro, 32
  solvent suppression, 228
pulse shape definitions, 36
pulse transmitter, 187
pulse width optimum, 188
Pulsed Field Gradient (PFG) experiments, 24
Pulsed Field Gradient (PFG) module, 196
puttxt command, 197
pw command, 188
pw parameter, 187, 188
pw90 parameter, 188
pwd command (UNIX), 37, 275
pwr command, 225

Q

qtune command, 116
quadrature detection, 227
  frequency shifted, 218
QUALITY menu, 162
quarter-wavelength cable, 114
question mark (?) notation, 96
queued operations, 30
queueing experiments, 200
quick transform, 72, 74
QuietJet Plus printer, 255
quitting Plot Designer, 271

R

r macro, 243
ra command, 202
radio-frequency emission regulations, 20
raw data storage, 31
rcp command, 282
Read All button, 89
Read button, 76
Read Text button, 76
readallshims macro, 136
readbrutape shell script, 290
readhw command, 132
README file, 38
readultra macro, 167
real channel, 224
real-time DSP, 210, 213
recalling
  command line entries, 97
  display parameters, 243
receiver gain, 206
receiver gating, 191
receiver gating times, 188
receiver overload, 205
Redisplay button, 82
Redraw button, 74
reduce size of graphics window, 47
Reference button, 79, 80
reference frequency, 247
reference in both dimensions, 80
reference line, 247
reference position, 247
reffrq parameter, 247, 248
reflected power, 25
refpos parameter, 247
Region button, 77
region command, 250, 253
Regression 1 menu, 86
Regression 2 menu, 86
regression analysis, 86
regression.inp file, 86
Regrs button, 81
relative path, 38
relief valves warning, 19
remote acquisition, 207
remote file copy, 282
remote host busy, 286
remote host name, 282
remote interactive shimming, 207
remote node, 282
remote status module, 27, 43
remote tape, 291
removable quench tubes warning, 19
removing
  directories, 276
  files, 276
  floppy disk from drive, 291
  lock, 208
Rename button, 91
rename command, 276
renaming
  directories, 276
  files, 91
Reprocess button, 74, 77, 79
Reset button, 75
reset integral to zero, 253
Resets button, 73
resets button, 239, 241
Resize button, 47, 66
resolution enhancement, 72, 223

resolution enhancement function, 221, 222
resolv command, 222
Resolve button, 72
Results button, 85
resuming acquisition, 202
retrieving
    compressed FIDs, 293
    FID data in files, 279
    parameters from parameter file, 279
    previous shim values, 137
    shim settings, 279
Return button, 69
Return key, 22, 46, 97
rf channels, 24
rfband parameter, 184
rfchannel parameter, 184
rfl parameter, 247
rfp parameter, 247
Right button, 78, 79
right button of mouse, 42
right command, 250
right half of the screen/page, 78, 79
right mouse button, 91
right phase, 224
right-arrow key, 97
rl command, 247
rm command, 276
rmdir command, 276
ROESY button, 69
rof1 parameter, 188
rof2 parameter, 187, 188, 216
room-temperature shim coil currents, 135
room-temperature shims adjustment, 168
root directory, 34, 37
root user, 36
root-mean-square noise, 246
Rotate button, 80
rotate spectral data, 80
rotating frame NOE 2D correlation, 69
rp parameter, 224, 225, 240
rsh command, 282
rt command, 279, 287
rtcmx command, 280
rtp command, 109, 279
rts command, 138, 279
rtv command, 279

S

s macro, 243
S2PUL button, 69
s2pul macro, 185
S2PUL pulse sequence, 185
sa command, 202
safety precautions, 17, 19
sample
    ejection, 103, 150
    height, 102, 145
    insertion, 25, 103, 105, 150
    position, 102
    preparation, 101
    spinning, 127, 128, 161
    tubes, 103
sample changer
    changing samples, 106
    sample position, 102
sample macro, 106
SAMPLE menu, 150, 151
sampling rate, 185
saturated lock signal, 139
saturation of the lock signal, 163
save button, 83
Save FID button, 90
Save Params button, 90
Save Shims button, 90
saving
    compressed FID, 292
    display parameter set, 243
    experiment data, 277
    FID data, 90
    parameters from current experiment, 90
    shim settings, 90, 278
sb button, 72, 223
sb parameter, 221
sbs button, 72, 223
sbs parameter, 221
sc parameter, 232, 236, 250
sc wc button, 243
sc2 parameter, 250
Scale button, 78
scale image to full window, 250
scale integral value, 253
scaling constant, 202
scientific notation arguments, 94
scroll bar, 47
scrollable window, 44, 45
SCSI high-speed link, 24
sd macro, 185
sd2 macro, 185
sd2a macro, 185
sd3 macro, 185
sd3a macro, 185
sda macro, 185
search spectrum for peaks, 185
second cursor, 42, 234
second Fourier transformation, 74
Secondary Main menu, 60, 91
second-level menus, 66
Select button, 83
Select Params button, 71, 73
Select Plotter button, 92
Select Printer button, 92, 271
seqfil experiment time, 189
seqfil parameter, 185
seqlib directory, 36
sequence, 70
Sequence button, 67
sequential execution of commands, 94
sequential sampled data, 227
serial communications, 34
set cursor position to zero, 79
Set Default button, 88
Set Directory button, 87
set display, 78, 79
Set Int button, 76
set nucleus, 68
Set Params button, 83
set solvent, 68

setallshims macro, 136
setfrq command, 183
sethw command, 124, 132
setint macro, 253
setoffset macro, 249
setpen macro, 255
setplotdev macro, 257
setref macro, 248
setref1 macro, 249
setref2 macro, 249
sets integral value, 253
setsw macro, 185
Setup button (GLIDE), 55, 66
setup macro, 68, 111
Setup menu, 67
sf parameter, 232
sf wf button, 71, 234
sfrq parameter, 24, 152, 183, 247
Sh All button, 77
Sh Box button, 76
Sh Lbl button, 77
Sh Pk button, 76
shaped pulses, 189
shapelib directory, 36
shared use of an experiment, 207
shell command, 207
shell in UNIX, 91
Shell Tool program, 50
shell windows, 48
shim adjust, 159
shim button (acqi program), 149, 159
shim coil diagram, 142
shim coil settings, 137, 278
shim coils, 135
shim combinations, 162
shim command, 138, 139, 144, 145, 200
shim directory, 90
shim gradient combinations, 141
shim menu, 161
shim method, 140
shim methods files, 36
shim parameters adjustment, 156
shim sets, 137
shim settings, 279
shim settings sets, 36
shim systems, 24
shim values, 136
SHIM window, 201
shimmaps
  displaying, 170
  distributing to users, 172
  loading, 172
shimmethods directory, 36, 139, 140, 145
shimmethods file, 139
shimming
  acquisition time, 140
  background Autoshim, 145
  criterion, 139, 140, 162
  lock signal effect, 139
  methods, 139, 140
  on FID, 160
  on spectrum, 160
  on the lock, 162
  quality, 139
  routine basis, 147
  shimming mode, 161
  user-defined shim methods, 142
shims controls, 156
shims directory, 36, 138, 278
shimset parameter, 132, 136, 141
shimspath parameter, 138, 278, 279
ShNum button, 76
Show Fit button, 85
Show Output Devices button, 92, 271
Show Params button, 83
Show Shims button, 90
Show Time button, 70
showplotq macro, 255
showplotter macro, 257
Silicon Graphics (SGI) workstation, 25, 290
simple Autolock, 132, 151
simple locking, 153
Simulate button, 83
Simulation button, 81
simultaneous access to files, 206
simultaneously sampled data, 227
sine transform, 224
Sinebell button, 74
sinebell constant, 72, 221, 223
sinebell shift constant, 72, 221, 223
sinebell weighting, 74
Single button (acqi), 155
single quote (') notation, 95
single-pulse experiments, 114
six-spin system, 84
Size button, 77, 79
size of directory entries, 89
Sizes button, 89
slide control, 152
slw parameter, 85
SMALL button (acqi), 149
small command, 47
small graphics window, 46
snap spacing, controlling, 263
software libraries, 34
software simple Autolock, 132
Solaris computing environment, 33
solids high-power amplifiers caution, 20
solid-state echo pulse sequence, 69
Solvent button, 54
solvent parameter, 249
solvent peak suppression, 228
solvent presaturation experiments, 190
solvent selection, 101
Solvent Selection Menu, 110
Solvent Selection menu, 68
Solvent Subtraction, 226
solvent subtraction filtering, 228
solvent suppression pulse sequences, 228
solvent volumes, 102
solvents directory, 111
solvents file, 248
solvents selection, 110
solvinfo command, 248
sort directory entries, 89
source code files, 36
sovent frequency, 248
sp parameter, 232, 250

sp wp button, 73, 83, 239, 240, 243
spcfrq command, 247
spectra phasing, 224
spectra, positioning, 262
spectral
    display, 159, 225, 231, 243
    intensity, 223
    intensity control, 239
    line frequencies and amplitudes, 78
    phase parameters, 77
    plotting, 243
    referencing, 247
    starting frequency, 240
    vertical spectral display position, 232
    width, 187
    width adjustment, 240
    window size, 185
    windowing mode, 239, 240
spectrometer frequency reference, 247
spectrometer system units, 23
Spectrum button (acqi), 155
spin command, 127
spin menu, 151, 161
spin parameter, 127, 152
spin rate adjustment, 127, 128
spin simulation analysis menus, 83
Spin Simulation First Definition menu, 83
Spin Simulation Line Assignment menu, 85
Spin Simulation Main menu, 83
Spin Simulation Second Definition menu, 84
Spin Simulation Secondary menu, 84
Spin Simulation Third Definition menu, 84
spin speed interlock, 134
spin status, 151
Spin System button, 83
spinner command, 127, 129
spinner control, 127, 142
Spinner Control window, 127, 129
spinning regulation, 128
Spinsight data retrieval, 280
spline-fit baseline correction, 251
split macro, 250
sqcosin macro, 222
sqsinebell macro, 222
squared sinebell function, 221
squared x-axis scale, 86
squared y-axis scale, 86
sread command, 289, 290
ss parameter, 187, 188
ssecho button, 69
ssfilter parameter, 228
sslsfrq parameter, 228, 229
ssntaps parameter, 228
ssorder parameter, 228
Stacked Plot button, 80
standard 2-pulse experiment, 69
Standard button, 70
standard carbon experiment, 67
standard coil groupings, 142
standard decoupler pulse sequence, 69
standard parameter sets, 110
standard parameter sets for a nucleus, 36
standard proton experiment, 67
standard two-pulse sequence, 185, 190
STARS software package, 33
start button (acqi), 162
start of chart, 232
start of FID, 232
start of plot, 232
starting criterion for shimming, 140
starting Plot Designer, 262
status concept, 190
status line, 45
status window, 44
stdpar directory, 36, 107, 108, 111, 145
stdshm macro, 143
steady-state pulses, 188
steady-state transients, 187
STOP button (acqi), 162
stopping
    acquisition, 202
    jobs in plot queue, 255
    limNET server, 286
streaming tape directory, 89
string arguments, 94
string parameters, 94
stty command (UNIX), 97
su command (VNMR), 115, 136, 138
sub button, 83
Subtract button, 82
subtract spectrum from add/subtract experiment, 82
sulog file, 208
Summed button (acqi), 155
Sun computers, 23, 25
superconducting magnet, 25
svf command, 138, 277
svp command, 138, 278
svs command, 138, 278
sw parameter, 185, 187, 212, 217
swept-tune-type NMR probe tuning, 116
switchable probe caution, 193
symmetrization in 2D inadequate, 80
symmetrization in J-resolved 2D spectra, 80
synchronizing commands with experiment
    submission, 201
synchronous decoupler mode, 191
syshelppath parameter, 70
system messages, 45
system requirement for Plot Designer, 262
systemmenulibpath parameter, 70

T

T shimming criterion, 140
T1 Analysis button, 81
T_1 data set, 81
T_1 of deuterated lock solvent, 130
T1 Proc button, 81
T_1 value, 81
T2 Analysis button, 81
T_2 data set, 81
T2 Proc button, 81
T_2 value, 81
tape archive, 289
tape command, 290
tape operations on a network, 291
tape parameter, 89
tar command (UNIX), 289, 291, 293

tcl directory, 47
Tcl version of dg window, 47
temp command, 195
temp parameter, 31, 196
temperature control window, 196
temperature cutoff point, 196
template, loading a Plot Design, 264
terminal acquisition, 207
tests directory, 107, 108
text command, 32, 94, 197, 278
text files, 37, 278
  editor, 197
  format, 286
  plotting, 262
  printing, 271
text window, 271
  uncover or conceal, 65
textvi command, 197
Th button, 73, 239
th parameter, 78
thadj macro, 246
ThinkJet printer, 255
third rf channel parameters, 109
three-spin system, 83
thumbwheel switches, 184
tight shimming criterion, 140, 162
time macro, 189
time to run an experiment, 189
time-domain data, 227
time-shared decoupling, 191
tin parameter, 196
tip-angle resolution, 194
tlt parameter, 241, 252
tmove macro, 226
TMS line, 248
TMS referencing, 110
tmsref macro, 248, 249
tn parameter, 68, 183, 185
TOCSY button, 70
tof parameter, 152, 183, 184, 185
total correlation 2D, 70
tpwr parameter, 190
tpwrf parameter, 191, 193
tpwrm parameter, 191, 193
Trace button, 74
Trace label, 156
Transform button, 71
Transform F2 button, 73
transformed spectrum storage, 31
transients completed, 49
transmitter
  attenuation, 191
  fine power control, 191
  offset, 184
  power, 190
transmitter nucleus parameter, 68
traymax parameter, 106
tree structure file system, 34
trigonal symmetrization, 80
tune command, 115
TUNE INTERFACE unit, 25, 115
tuneoff macro, 124, 125, 126
tuning gain knob, 25
tuning meter, 25
tuning rods, 25
tuning selector switch, 25
two-spin system, 83

U

Ultra•nmr shim system II, 24
Ultra•nmr Shims, 164–168
  floppy disk use, 166
  interface box, 164
  power down, 167
  power on, 167
  shimming, 166
umount command (UNIX), 291
uncompress command (UNIX), 293
unit command, 95
UNITY*plus* spectrometer
  decoupler modes, 190
  linear modulators, 193
  lock frequency, 184
  probe tuning, 115
UNIX
  convert file from VXR-style, 286
  file security, 284
  file system, 34
  floppy disk as a file system, 291
  printing utilities, 271
  shell, 91
  system administrator, 36
UNIX button, 91
unix_vxr command, 286
unix2dos command (UNIX), 291
unlock command, 207, 208
unlocked experiments, 132
Unmark button, 76
up button, 155
up-arrow key, 97
update old parameter characteristics, 109
updatepars macro, 280
upper barrel warning, 18
use fitspec button, 85
Use Line List button, 85
use ll button, 85
Use Mark button, 85
user directories, 36
user group library, 38
user library, 38
user name assignment, 39
user-contributed files, 36
userfixpar macro, 110
usergo macro, 198
userlib directory, 36, 38
userplc macro, 250
userplh macro, 249
user-selected shim methods, 142
user-written weighting functions, 222
usr directory, 34

V

variable temperature (VT) accessory, 195, 196
variable temperature status, 43
Varian NMR software program, 25
VAX computer, 281

version of parameter set, 280
vertical scale, 42
vertical scale adjustment, 77
vertical scale of display, 232
vertical scaling modes, 245
vertical scaling multiplies, 159
vf parameter, 223, 232, 234
View button, 77
VNMR
  display screen, 27
  entering, 39
  exiting, 40, 51
  menu system, 59
  software, 25
  system directory, 88
  systems, 281
  user directory, 88
vnmr directory, 34, 36
VNMR Online hypertext manual, 34, 50
VNMR shell window, 48
vnmr1 directory, 36
vnmr1 user, 36
vnmreditor variable, 197
VnmrI, 25, 290
vnmrplot command, 255
vnmrprint command, 271
VnmrSGI, 25, 290
vnmrsys directory, 36, 37
vnmrtext variable (UNIX), 48
VnmrX, 25
vo parameter, 237
volmgt program, 291
Volume button, 75
vp parameter, 232, 240, 245
vpf parameter, 232, 234, 236
vpfi parameter, 234
Vproj (max) button, 75
Vproj (sum) button, 75
vs parameter, 223, 232, 239
vsadj macro, 245
vsadj2 command, 245
vsadjc macro, 245
vsadjh macro, 245
VT experiment warning, 18
VT status, 152
vtc parameter, 196
vttype parameter, 151, 205
VXR library file extraction, 287
vxr_unix command, 287
VXR-4000 systems, 281
VXR-S systems, 281
VXR-style systems, 281
VXR-style tape, 290

W

walkup NMR, 58
Walkup NMR Using GLIDE manual, 58
WALTZ-16 decoupling, 193, 194, 195
warnings defined, 17
water suppression, 69, 147
waveform generator accessory, 24
waveform generator programmable decoupling, 194
wbs command, 204
wbs parameter, 71, 204, 208
wc parameter, 232, 236, 250
wc2 parameter, 250
wc2max parameter, 255, 256, 257
wcmax parameter, 255, 256, 257
weight and Fourier transform, 71, 221
weight, Fourier transform, phase each FID, 81
Weight, Transform button, 71
weighting function, 221–223
  user-written, 222
weighting parameters, 72
werr command, 203
werr parameter, 203, 204, 208
wexp command, 204
wexp parameter, 71, 203, 204, 208
wf parameter, 232
wft command, 204, 221, 223, 227
whitewashed FIDs, 237
width of chart, 232
width of FID, 232
width of plot, 77, 232
Wilmad tubes, 102
window closing and opening, 50
windows on display screen, 27, 44
wnt command, 204
wnt parameter, 71, 204, 208
working directory, 37, 38
Workspace button, 66
Workspace Menu, 49
workspace part of screen, 28
wp parameter, 232, 250
Write button, 89
Write Pulse Sequence button, 91
Write Text button, 76
writefid command, 278
wshim parameter, 139, 144, 154, 176, 207
wtfile parameter, 222
wti command, 72, 223
wysiwyg parameter, 232, 250

X

X and Y radial shim gradients, 136
X Window System, 25
x0 parameter, 262
x1 button (acqi), 156
x1 parameter, 136
X1 shim gradient, 136
XL systems, 281
x-linear button, 86
x-log button, 86
XPOLAR button, 69
x-square button, 86
XY32 decoupling, 194

Y

y0 parameter, 262
y-linear button, 86
y-log button, 86
ypcat command (UNIX), 282
y-square button, 86

Z

Z axial shim gradient, 135
z command, 253
Z0 field offset coil, 136
Z0 field position, 132
z0 parameter, 136, 152, 184
Z1 and Z2 adjustment, 163
z1 parameter, 136
Z1 room temperature shim as a gradient, 174
Z1 shim gradient, 136
Z1 shimming hardware, 146
z1c parameter, 136
z2 parameter, 136
Z2 shim gradient, 136
z2c parameter, 136
Z3 and Z4 adjustment, 163
zero and first order baseline correction mode, 241
zero filling, 72, 74
Zero Imag button, 71, 234
zero point of ADC, 155
zero-filling, 224
zero-frequency suppression, 228
zero-order baseline correction, 241, 252
zero-order FID phasing constant, 226
Zeta plotter, 254
zfs (zero-frequency suppression), 228
zoom macro, 250

Index